



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 173736

TO: Ben Sackey
Location: rem-5b31/5c18
Art Unit: 1626
December 9, 2005

Case Serial Number: 10/673988

From: P. Sheppard
Location: Remsen Building
Phone: (571) 272-2529

sheppard@uspto.gov

Search Notes

FOR OFFICIAL USE ONLY

173736

ACCESS DB #

PLEASE PRINT CLEARLY

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: BEN SACKETT Examiner #: 73489 Date: 12/8/05
Art Unit: 1826 Phone Number: 2-0704 Serial Number: 10/673,988
Location (Bldg/Room#): REM 5B31 (Mailbox #): C18 Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Method of producing alkoxy malonamides
Inventors (please provide full names): Bartek et al

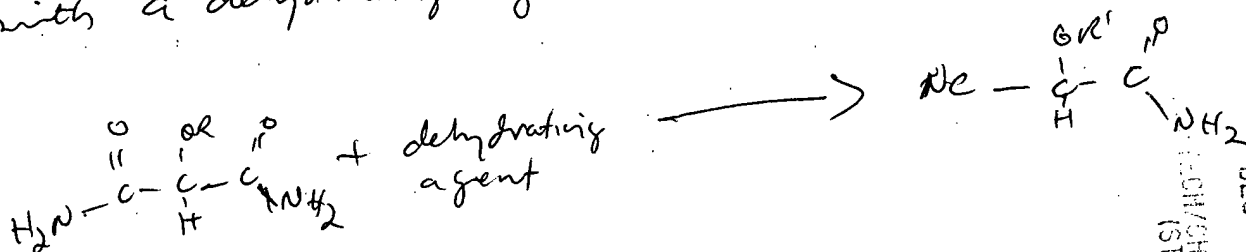
Earliest Priority Date: 5/6/00

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

A process for preparing 2-cyano-2-alkoxyacetamides of formula (III):
Comprising reacting alkoxy malonamides of formula (II) with a dehydrating agent:



RECEIVED
DEC - 8 2005
SCM/STET CIVIL-11
(STIC)

eg of dehydrating agents

trichloroacetic anhydride
di-butyltin oxide, phosphorus oxychloride
phosphorus trichloride

Sackey 10_673988- - History

=> d his ful

(FILE 'HCAPLUS' ENTERED AT 16:19:52 ON 09 DEC 2005)

FILE 'REGISTRY' ENTERED AT 16:58:12 ON 09 DEC 2005

L1 STR
L3 31 SEA SSS FUL L1
L6 STR
L8 158 SEA SSS FUL L6
L9 49 SEA ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN OR DIBUTYLTIN
OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR PHOSPHORUS
TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
L11 643 SEA ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN

FILE 'HCAPLUS' ENTERED AT 17:06:09 ON 09 DEC 2005

L12 8 SEA ABB=ON PLU=ON L3
D STAT QUE
D IBIB ABS HITSTR L12 1-8
L13 70 SEA ABB=ON PLU=ON L8
L14 25437 SEA ABB=ON PLU=ON L9 OR TRIFLUOROACETIC(W) ANHYDRIDE OR
DIBUTYLTIN(W) OXIDE OR PHOSPHORUS(W) (OXYCHLORIDE? OR TRICHLORID
E OR PENTACHLORIDE?)
L15 73122 SEA ABB=ON PLU=ON L11 OR ALUMINUM (W) CHLORIDE OR ALCL3
L16 389244 SEA ABB=ON PLU=ON ("DEHYDRATION AGENTS"/CV OR "DEHYDRATION
REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR DEHYDRAT? OR
DRYING
L17 30094 SEA ABB=ON PLU=ON ("LEWIS ACIDS"/CV OR "CARBONYLS (L) LEWIS
ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/CV OR
ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV) OR
LEWIS(W) ACID
L20 4 SEA ABB=ON PLU=ON (L8 AND (L16 OR L14 OR L17 OR L15)) NOT
L12
L21 1744 SEA ABB=ON PLU=ON CYANO(L)?ACETAMIDE?
L22 1 SEA ABB=ON PLU=ON (L21 AND L13) NOT L12
L23 5 SEA ABB=ON PLU=ON L20 OR L22
D STAT QUE
D IBIB ABS HITSTR L23 1-5
L24 62 SEA ABB=ON PLU=ON ("BARTEK J"/AU OR "BARTEK J P"/AU) OR
"BARTEK JOHANNES"/AU
L25 222 SEA ABB=ON PLU=ON ("FUCHS R"/AU OR "FUCHS R A"/AU OR "FUCHS
R E M"/AU OR "FUCHS R F"/AU OR "FUCHS R J"/AU OR "FUCHS R
K"/AU OR "FUCHS R L"/AU OR "FUCHS R M"/AU OR "FUCHS R P"/AU OR
"FUCHS R P P"/AU OR "FUCHS R R"/AU OR "FUCHS R WAYNE"/AU) OR
"FUCHS RUDOLF"/AU
L26 15 SEA ABB=ON PLU=ON "HILDBRAND STEFAN"/AU
L27 14 SEA ABB=ON PLU=ON L26 NOT (L12 OR L20)
D STAT QUE L27 NOS
D IBIB ABS L27 1-14
L29 0 SEA ABB=ON PLU=ON ((L24 OR L25) AND L13) NOT (L12 OR L20 OR
L27)
L30 5603 SEA ABB=ON PLU=ON (L16 OR L14) AND (L17 OR L15)

FILE 'REGISTRY' ENTERED AT 17:17:32 ON 09 DEC 2005

L31 1285 SEA ABB=ON PLU=ON MALONAMIDE?

FILE 'HCAPLUS' ENTERED AT 17:17:57 ON 09 DEC 2005

L32 3721 SEA ABB=ON PLU=ON L31 OR ?MALOMAMIDE?
L33 8 SEA ABB=ON PLU=ON L32 AND L30
L34 7 SEA ABB=ON PLU=ON L33 NOT (L12 OR L20 OR L27)
D STAT QUE L29

Sackey 10_673988- - History

D STAT QUE L34
D IBIB ABS HITSTR L34 1-7

L35 FILE 'CASREACT' ENTERED AT 17:26:39 ON 09 DEC 2005
L36 0 SEA SSS SAM L1 (0 REACTIONS)
2 SEA SSS FUL L1 (35 REACTIONS)
D STAT QUE
D IBIB ABS RXS 1-2

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 DEC 2005 HIGHEST RN 869627-02-1
DICTIONARY FILE UPDATES: 8 DEC 2005 HIGHEST RN 869627-02-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE HCAPLUS

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FILE COVERS 1907 - 9 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 8 Dec 2005 (20051208/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

Sackey 10_673988- - History

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CASREACT

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FILE CONTENT:1840 - 4 Dec 2005 VOL 143 ISS 23

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*

* CASREACT now has more than 10 million reactions *

*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 17:06:09 ON 09 DEC 2005

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 9 Dec 2005 VOL 143 ISS 25

FILE LAST UPDATED: 8 Dec 2005 (20051208/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

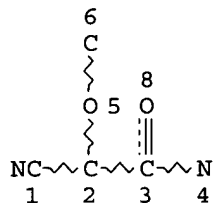
This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d stat que

L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L3 31 SEA FILE=REGISTRY SSS FUL L1

L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=>

=>

=> d ibib abs hitstr l12 1-8

L12 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:804106 HCAPLUS

DOCUMENT NUMBER: 142:23494

TITLE: Three-Component Condensation Leading to β -Amino Acid Diamides: Convergent Assembly of β -Peptide Analogues

AUTHOR(S): Oaksmith, Jennifer M.; Peters, Ulf; Ganem, Bruce

CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University, Ithaca, NY, 14853-1301, USA

SOURCE: Journal of the American Chemical Society (2004), 126(42), 13606-13607
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

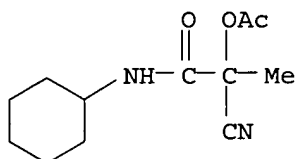
OTHER SOURCE(S): CASREACT 142:23494

AB A Passerini condensation of acyl cyanides, carboxylic acids, and isonitriles has been developed that affords efficient access to functionalized diamides as well as β -peptides of α -hydroxy- β -amino acids. Such compds. are protease-resistant and form stable helical and sheet structures when incorporated into larger peptides (no data given). N-Protected α -amino acids and isocyanooesters derived from α -amino acids participate in the condensation, leading to α/β peptides embodying the heterogeneous $\alpha/\beta/\alpha$ backbone motif.

IT 799778-66-8P 799778-69-1P 799778-85-1P
799778-93-1P 799779-04-7P 799779-09-2P
799779-13-8P 799779-16-1P 799779-25-2P
799779-30-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (acyloxy)(cyano)carboxamides via via Passerini condensation of acyl cyanides, carboxylic acids, and isonitriles)

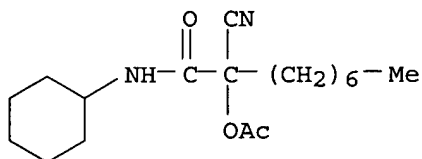
RN 799778-66-8 HCAPLUS

CN Propanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)



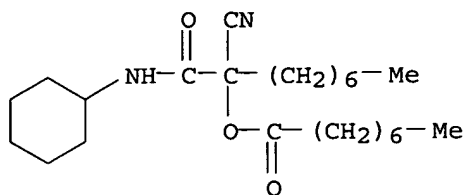
RN 799778-69-1 HCAPLUS

CN Nonanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)

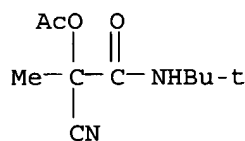


RN 799778-85-1 HCAPLUS

CN Octanoic acid, 1-cyano-1-[(cyclohexylamino)carbonyl]octyl ester (9CI) (CA INDEX NAME)

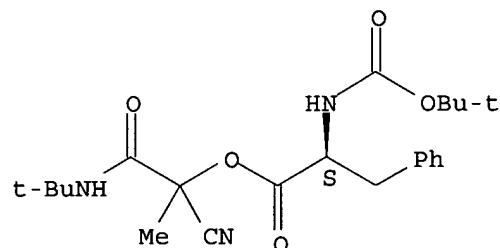


RN 799778-93-1 HCAPLUS
 CN Propanamide, 2-(acetyloxy)-2-cyano-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

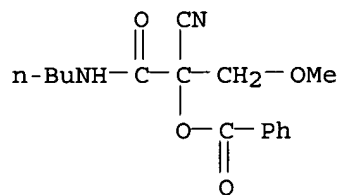


RN 799779-04-7 HCAPLUS
 CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, 1-cyano-2-[(1,1-dimethylethyl)amino]-1-methyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

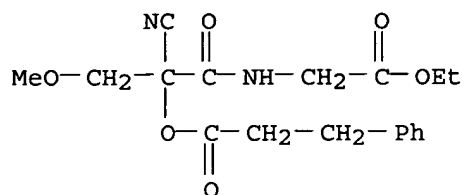
Absolute stereochemistry.



RN 799779-09-2 HCAPLUS
 CN Propanamide, 2-(benzoyloxy)-N-butyl-2-cyano-3-methoxy- (9CI) (CA INDEX NAME)

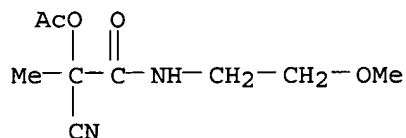


RN 799779-13-8 HCAPLUS
 CN Benzenepropanoic acid, 1-cyano-2-[(2-ethoxy-2-oxoethyl)amino]-1-(methoxymethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)



RN 799779-16-1 HCAPLUS

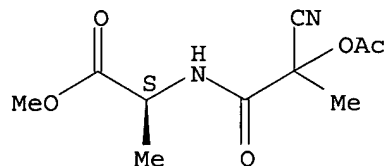
CN Propanamide, 2-(acetyloxy)-2-cyano-N-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



RN 799779-25-2 HCAPLUS

CN L-Alanine, N-[2-(acetyloxy)-2-cyano-1-oxopropyl]-, methyl ester (9CI) (CA INDEX NAME)

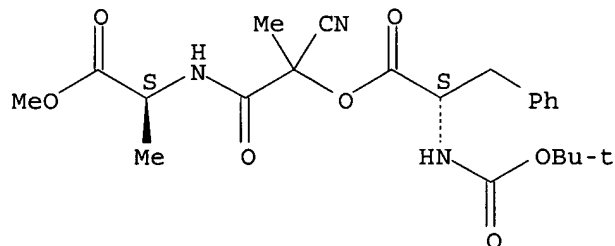
Absolute stereochemistry.



RN 799779-30-9 HCAPLUS

CN 3,8-Dioxa-5,11-diazatridecan-13-oic acid, 9-cyano-2,2,9,12-tetramethyl-4,7,10-trioxo-6-(phenylmethyl)-, methyl ester, (6S,12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



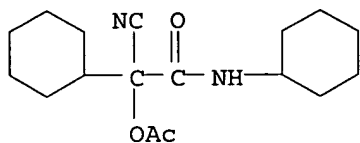
IT 799778-72-6P 799778-75-9P 799778-78-2P
799778-81-7P 799778-83-9P 799778-88-4P
799778-90-8P 799778-98-6P 799779-01-4P
799779-07-0P 799779-11-6P 799779-19-4P
799779-22-9P 799779-28-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of (acyloxy)(cyano)carboxamides via via Passerini condensation
of acyl cyanides, carboxylic acids, and isonitriles)

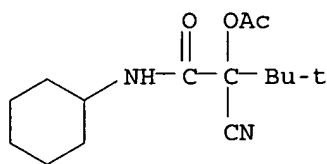
RN 799778-72-6 HCAPLUS

CN Cyclohexaneacetamide, α -(acetyloxy)- α -cyano-N-cyclohexyl-
(9CI) (CA INDEX NAME)



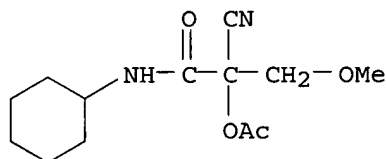
RN 799778-75-9 HCAPLUS

CN Butanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl-3,3-dimethyl- (9CI) (CA
INDEX NAME)



RN 799778-78-2 HCAPLUS

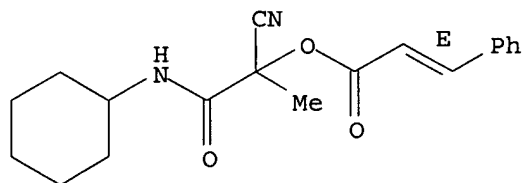
CN Propanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl-3-methoxy- (9CI) (CA
INDEX NAME)



RN 799778-81-7 HCAPLUS

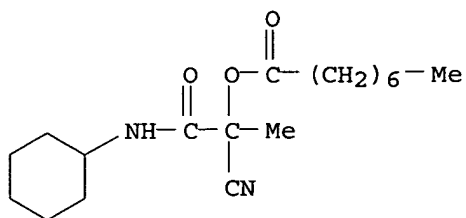
CN 2-Propenoic acid, 3-phenyl-, 1-cyano-2-(cyclohexylamino)-1-methyl-2-
oxoethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



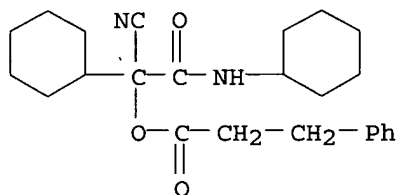
RN 799778-83-9 HCAPLUS

CN Octanoic acid, 1-cyano-2-(cyclohexylamino)-1-methyl-2-oxoethyl ester (9CI)
(CA INDEX NAME)



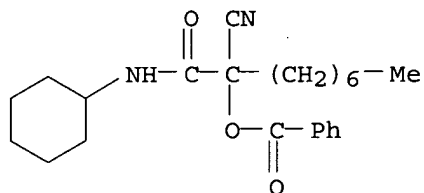
RN 799778-88-4 HCAPLUS

CN Benzenepropanoic acid, 1-cyano-1-cyclohexyl-2-(cyclohexylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



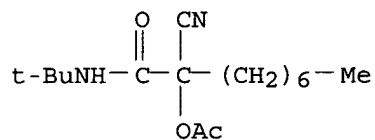
RN 799778-90-8 HCAPLUS

CN Nonanamide, 2-(benzyloxy)-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)



RN 799778-98-6 HCAPLUS

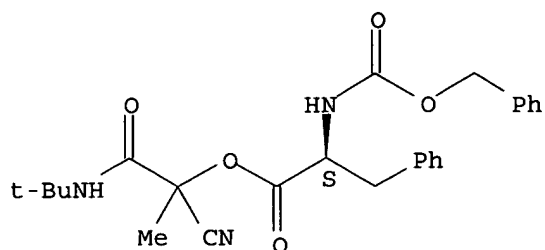
CN Nonanamide, 2-(acetyloxy)-2-cyano-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



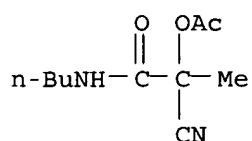
RN 799779-01-4 HCAPLUS

CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]-, 1-cyano-2-[(1,1-dimethylethyl)amino]-1-methyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

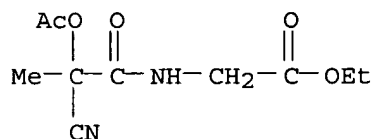
Absolute stereochemistry.



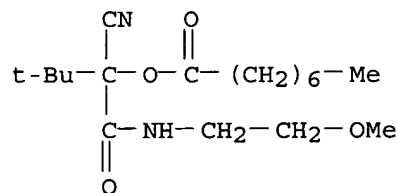
RN 799779-07-0 HCAPLUS
CN Propanamide, 2-(acetyloxy)-N-butyl-2-cyano- (9CI) (CA INDEX NAME)



RN 799779-11-6 HCAPLUS
CN Glycine, N-[2-(acetyloxy)-2-cyano-1-oxopropyl]-, ethyl ester (9CI) (CA INDEX NAME)

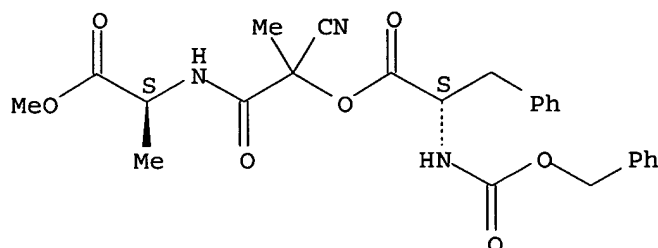


RN 799779-19-4 HCAPLUS
CN Octanoic acid, 1-cyano-1-[[2-(methoxyethyl)amino]carbonyl]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)



RN 799779-22-9 HCAPLUS
CN 2,7-Dioxa-4,10-diazadodecan-12-oic acid, 8-cyano-8,11-dimethyl-3,6,9-trioxo-1-phenyl-5-(phenylmethyl)-, methyl ester, (5S,11S)- (9CI) (CA INDEX NAME)

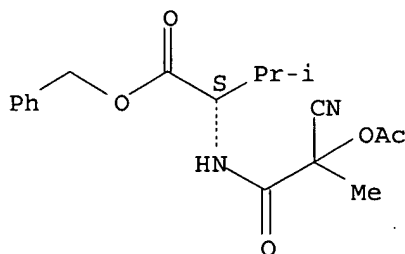
Absolute stereochemistry.



RN 799779-28-5 HCAPLUS

CN L-Valine, N-[2-(acetyloxy)-2-cyano-1-oxopropyl]-, phenylmethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:749510 HCAPLUS

DOCUMENT NUMBER: 138:32334

TITLE: Reactions of Mn(III) quadridentate Schiff base
compounds with TCNQ anion to form unusual TCNQ
derivatives by alcoholysisAUTHOR(S): Miyasaka, Hitoshi; Sugimoto, Kunihiisa; Sugiura,
Ken-Ichi; Ishii, Tomohiko; Yamashita, MasahiroCORPORATE SOURCE: Department of Chemistry, Graduate School of Science,
Tokyo Metropolitan University, Tokyo, 192-0397, Japan
SOURCE: Molecular Crystals and Liquid Crystals Science and
Technology, Section A: Molecular Crystals and Liquid
Crystals (2002), 379, 197-204

CODEN: MCLCE9; ISSN: 1058-725X

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reactions of Mn(III) quadridentate Schiff base compds.,
[Mn(saltmen)(H₂O)]ClO₄ (1; saltmen²⁻ = N,N'-(1,1,2,2-
tetramethylethylene)bis(salicylideneiminato)) and [Mn(naphtmen)(H₂O)]ClO₄
(2; naphtmen²⁻ = N,N'-(1,1,2,2-tetramethylethylene)bis(naphthylideneiminat
o)), with LiTCNQ gave three types of compds. depending on reaction
conditions: [Mn(saltmen)(H₂O)](TCNQ) (3), [Mn(saltmen)(MeOH)(TCNQ-OMe)]
(4, TCNQ-OMe⁻ = p-(α,α-dicyano-α-
methoxytolyl)dicyanomethanide), and [Mn(naphtmen)(MeOH)(TCNQA-OMe)] (5,
TCNQA-OMe⁻ = p-(α-cyano-α-methoxy-α-
methylamidotolyl)dicyanomethanide). Compds. 3·MeOH and 5 were
characterized by x-ray crystallog. Compds. 3 and 4 were prepared under

anaerobic and aerobic conditions, resp., in MeOH/H₂O. Compound 5 was synthesized under aerobic conditions analogous to 4. For 4 and 5, unusual addition reactions on the anionic TCNQ mol. occurred to form (TCNQ-OMe)- for 4 and (TCNQA-OMe)- for 5. Ferromagnetic and antiferromagnetic interactions in the prepared compds. were investigated.

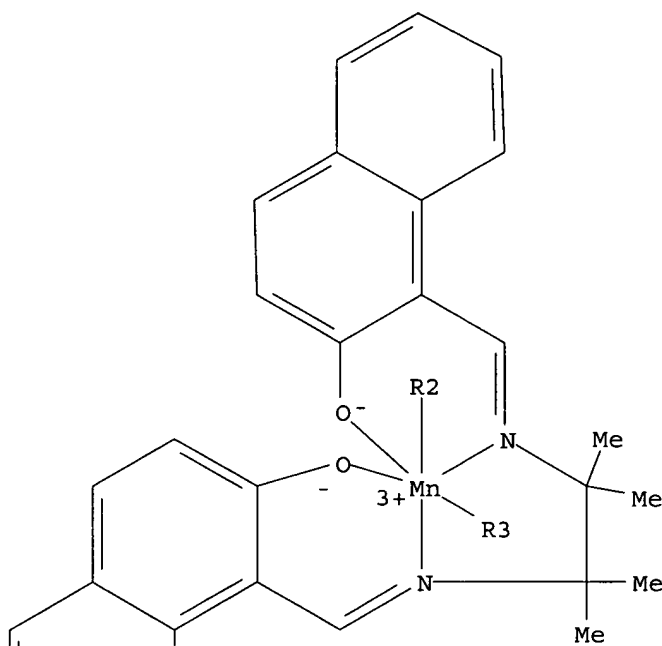
IT 478158-45-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and magnetic properties of)

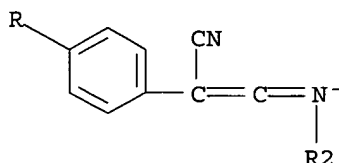
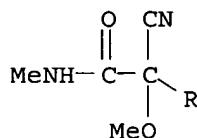
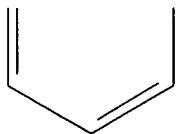
RN 478158-45-1 HCAPLUS

CN Manganese, [α -cyano-4-[1-cyano-2-(imino- κ N)ethenyl]- α -methoxy-N-methylbenzeneacetamidato] (methanol) [[1,1'-[(1,1,2,2-tetramethyl-1,2-ethanediyl)bis[(nitrilo- κ N)methylidyne]]bis[2-naphthalenolato- κ O]](2-)]-, (OC-6-34)- (9CI) (CA INDEX NAME)

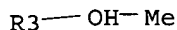
PAGE 1-A



PAGE 2-A



PAGE 3-A



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:597946 HCAPLUS
 DOCUMENT NUMBER: 135:152562
 TITLE: Dehydration method for producing 2-(alkoxy)malonodinitriles from 2-alkoxymalondiamides
 INVENTOR(S): Bartek, Johannes; Fuchs, Rudolf; Hildbrand, Stefan
 PATENT ASSIGNEE(S): Lonza A.-G., Switz.
 SOURCE: PCT Int. Appl., 13 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058857	A1	20010816	WO 2001-EP1505	20010209
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US, US, US			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

AU 2001033759	A5	20010820	AU 2001-33759	20010209
EP 1254105	A1	20021106	EP 2001-905765	20010209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003522753	T2	20030729	JP 2001-558409	20010209
US 2003144538	A1	20030731	US 2002-182716	20021011
US 6673957	B2	20040106		
US 2004063987	A1	20040401	US 2003-673988	20030930
PRIORITY APPLN. INFO.:			EP 2000-102758	A 20000210
			EP 2000-109505	A 20000504
			US 2001-267087P	P 20010207
			WO 2001-EP1505	W 20010209
			US 2002-182716	A3 20021011

OTHER SOURCE(S): CASREACT 135:152562; MARPAT 135:152562

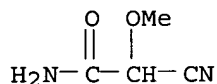
AB 2-(Alkoxy)malonodinitriles (NC)2CHOR (R = C1-6 alkyl, halogen-substituted C1-6 alkyl) (e.g., 2-methoxymalonodinitrile) or 2-(alkoxy)-2-cyanoacetamides are prepared by the dehydration of the corresponding 2-alkoxymalondiamides (H₂NCO)2CHOR in the presence of a dehydrating agent (e.g., POCl₃).

IT 353291-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(dehydration method for producing 2-(alkoxy)malonodinitriles from 2-alkoxymalondiamides)

RN 353291-71-1 HCAPLUS

CN Acetamide, 2-cyano-2-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:408241 HCAPLUS

DOCUMENT NUMBER: 115:8241

TITLE: Reactions of methoxynaphthalenes with active methylene compounds in the presence of manganese(III) acetate

AUTHOR(S): Tsunoda, Katsunori; Yamane, Mitsuyoshi; Nishino, Hiroshi; Kurosawa, Kazu

CORPORATE SOURCE: Fac. Sci., Kumamoto Univ., Kumamoto, 860, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1991), 64(3), 851-6

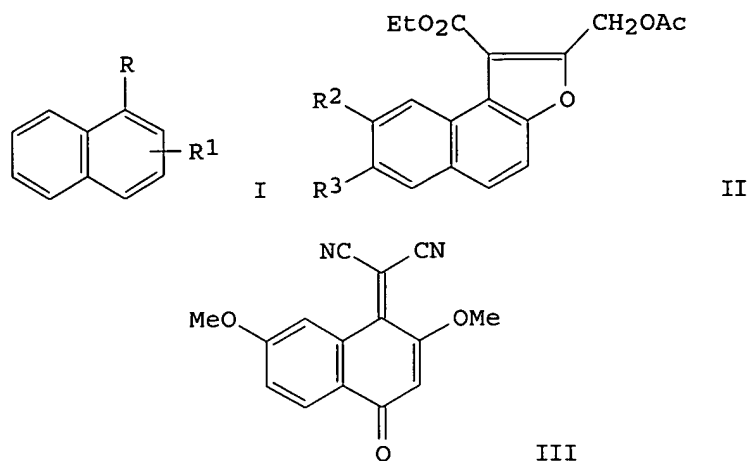
CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:8241

GI



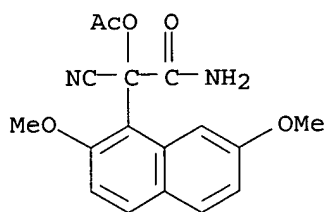
AB The reaction of methoxynaphthalenes I [R = H, R1 = 2-OMe, 4-OMe, 2,6-(OMe)2, 2,7-(OMe)2, 4,6-(OMe)2, 6,7-(OMe)2] with malonamide in the presence of manganese(III) acetate gave 2-acetoxy-2-(1-naphthyl)propanediamides I [R = C(OAc)(CONH2)2] and 2-hydroxy-2-(1-naphthyl)propanediamides I [R = C(OH)(CONH2)2]. The reaction of methoxynaphthalenes with Et 3-oxobutanoate, 2-cyanoacetamide, and malononitrile in the presence of manganese(III) acetate also yielded the corresponding substituted naphthalenes, Et 2-(acetoxymethyl)naphtho[furan-1-carboxylates II (R2, R3 = H, OMe), and/or a 4-methylnaphthalenone III. The reaction mechanisms are discussed.

IT 134255-39-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 134255-39-3 HCAPLUS

CN 1-Naphthaleneacetamide, α -(acetyloxy)- α -cyano-2,7-dimethoxy-
(9CI) (CA INDEX NAME)



L12 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:579018 HCAPLUS

DOCUMENT NUMBER: 87:179018

TITLE: Amino acid derivatives as fungicides

INVENTOR(S): Ishida, Yasuo; Yakushiji, Kunito; Wakae, Osamu; Aoki, Isao; Masumoto, Keiichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

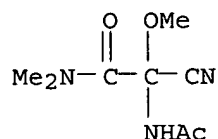
CODEN: JKXXAF

DOCUMENT TYPE: Patent

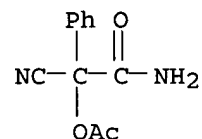
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 52021327	A2	19770217	JP 1975-97931	19750811
PRIORITY APPLN. INFO.:				JP 1975-97931	A 19750811
AB	Amino acid derivs. are used as microbicides. Thus, N,N,-dimethyl-2-acetamido-2-cyano-2-(propylthio)acetamide [PrSC(CN)(NHAc)CONMe2] [64205-24-9] sprayed on tomatoes at 250 ppm almost completely controlled Phytophthora infestans infection. This compound and 28 its analogs were prepared and their fungicidal activities presented.				
IT	64205-28-3P RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and fungicidal activity of)				
RN	64205-28-3 HCAPLUS				
CN	Acetamide, 2-(acetylamino)-2-cyano-2-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)				



L12 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1968:12238 HCAPLUS
 DOCUMENT NUMBER: 68:12238
 TITLE: Cyanide-catalyzed fragmentation of triketone monoximes
 AUTHOR(S): Crabtree, Eleanor V.; Poziomek, Edward J.
 CORPORATE SOURCE: Edgewood Arsenal, Edgewood, MD, USA
 SOURCE: Journal of Organic Chemistry (1967), 32(4), 1231-3
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB 1-Phenyl-1,2,3-butanetrione 2-oxime (I) is treated with KCN to give 2-cyano-2-hydroxy-2-phenylacetamide (II); N.M.R. data for II are given. The I-CN- reaction is inhibited by PhCOCONH2; CN- catalyzes the cleavage of I.
 IT **7616-88-8P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 7616-88-8 HCAPLUS
 CN Mandelamide, α-cyano-, acetate (ester) (8CI) (CA INDEX NAME)



L12 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

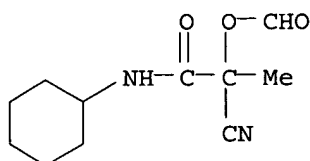
ACCESSION NUMBER: 1966:465427 HCAPLUS
 DOCUMENT NUMBER: 65:65427
 ORIGINAL REFERENCE NO.: 65:12170c-e
 TITLE: Heterocyclic isonitriles
 AUTHOR(S): Neidlein, R.
 CORPORATE SOURCE: Univ. Marburg/Lahn, Germany
 SOURCE: Arch. Pharm (1966), 299(7), 603-5
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 65:65427

AB The preparation of 3-isonitrilopyridine (I) and α -furfurylisonitrile (II) and their reactions with carboxylic acids, ketones, and amines to give the corresponding acylaminocarboxamides are described. Acyl cyanides with isonitriles and carboxylic acids yielded the corresponding α -hydroxy- α -cyanocarboxamides. 3-Formamidopyridine (12.2 g.) in 32 cc. Et₃N and 150 cc. CH₂Cl₂ treated with stirring and cooling with 9.9 g. COCl₂ and then with 50 cc. saturated aqueous Na₂CO₃ yielded 7.3 g. I. N-Formyl- α -furfurylamine (12.5 g.), 32 cc. Et₃N, and 9.9 g. COCl₂ gave similarly II. Cyclohexanone (5.4 g.) and 3.5 g. iso-PrNH₂ treated slowly with cooling with 5.2 g. crude I in 25 cc. iso-PrOH and 2.6 cc. HCO₂H and kept 4 hrs. gave 4.2 g. 1-(N-formylisopropylamino)cyclohexane-1-carboxylic acid 3-pyridylamide (III), m. 180-1° (MeCN). II (5.4 g.), 3.5 g. iso-PrNH₂, and 54 g. cyclohexanone in 15 cc. PrOH treated at -30° with 2.6 g. HCO₂H in portions yielded 4.5 g. α -furfurylamide analog of III, m. 137-8° (EtOH). Cyclohexyl isocyanide (5.45 g.) treated with cooling with 3.8 g. AcCN and then with 2.6 g. HCO₂H in portions yielded 6.5 g. 2-cyano-2-formyloxypropionic acid cyclohexylamide, m. 123-4° (EtOH-petr. ether).

IT 91430-76-1, Lactamide, 2-cyano-N-cyclohexyl-, formate
 (preparation of)

RN 91430-76-1 HCAPLUS

CN Lactamide, 2-cyano-N-cyclohexyl-, formate (7CI) (CA INDEX NAME)



L12 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1964:424911 HCAPLUS
 DOCUMENT NUMBER: 61:24911
 ORIGINAL REFERENCE NO.: 61:4210g-h,4211a-d
 TITLE: Reactions between isonitrosoacetone and hydrocyanic acid
 AUTHOR(S): Nenz, A.; Marangoni, L.; Gallinella, E.; Iliceto, A.
 CORPORATE SOURCE: Soc. Edison, Milan
 SOURCE: Chimica e l'Industria (Milan, Italy) (1964), 46(5), 509-17

CODEN: CINMAB; ISSN: 0009-4315

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 61:24911

AB RCOCH:NOH (I) (R = Me), HCN, and a catalyst (piperidine, KOH, KCN, NaCN) were mixed at the rate 1:0.32:0.01 by weight, 5.5 parts of an inert solvent

(CCl₄ or C₂H₄Cl₂) added, the mixture kept in a closed vessel, with stirring, at 30°, 30-80 hrs., the solvent and residual HCN decanted or dist., the residue extracted with Et₂O, and the resulting crude product recrystd. in CHCl₃/EtOH (95:5) to give RC(CN)(OH)CONH₂ (II) (R = Me, IIa), m. 85-6°. In a similar way the following II were prepared [R, Hcn:I ratio, solvent, reaction temperature, time (hrs.), % yield, and m.p. given]: Et (III), 1, CCl₄, 30°, 80, 39.6, 75-6°; iso-Bu (IV), 1, -, 30°, 70, 70.3, 84-5°; Ph (V), 2.4, CCl₄, 20°, 190, 46.5, 91-2°; p-O₂NC₆H₄ (VI), 2, CCl₄, 20°, 140, 83.9, 149-50°. I (R = p-MeC₆H₄ and p-MeOC₆H₄) gave, under the same conditions, only p-MeC₆H₄CO₂H and p-MeOC₆H₄CO₂H, resp. MeC(CN)(OH)CH:NOH (VII) (5 g.) was kept at 30° in a closed vessel 4 days and taken up in 10 ml. Et₂O and the solvent evaporated to give 2.8 g. crude IIa. To 5 g. VII in 20 ml. anhydrous Et₂O 1.8 g. HCl gas was introduced at -15° the mixture kept at this temperature 3 hrs., the solvent evaporated, and the product dried

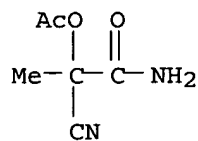
at

-25° during 4 hrs. to give 3.2 g. IIa. AcCONH₂ (5 g.) was added with stirring to a mixture of 27 g. CCl₄, 1.6 g. HCN, and 0.05 g. piperidine, after 5 min. the solvent was evaporated, a few ml. Et₂O and 40 ml. boiling CHCl₃ added, and the mixture worked up to give 3 g. IIa. II (10 g.) was dissolved in 62 g. 97.2% H₂SO₄, at 0-20° and kept overnight at room temperature, the solution poured into 500 ml. Et₂O, the precipitate taken

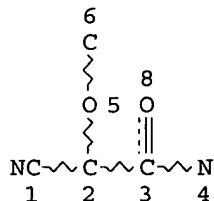
up in 70

ml. EtOH, and the solution worked up to give 9.4 g. MeC(OH)(CONH₂)₂ (VIII), m. 211-12°. IIa (10 g.) was dissolved in 20 ml. concentrated HCl, keeping the temperature below 65°, left overnight at room temperature, and extracted 10 times with 50 ml. Et₂O, and the solution worked up to give 6.2 g. MeC(OH)(CO₂H)₂ (IX), m. 140° (H₂O). IIa (10 g.) was dissolved in 17 g. 100% H₂SO₄, keeping the temperature below 60°, heated 1 hr. at 100°, and cooled to 60°, 11.2 g. MeOH added, the mixture heated 15 hrs. at 90°, 60 ml. anhydrous Et₂O added, and the solution worked up to give 9.7 g. MeC(OH)(CO₂Me)₂ (X), b₃ 71°, n_{20D} 1.4287. To 30 g. IIa in 100 ml. Ac₂O, 0.1 g. C₅H₅N was added and the mixture heated 100 min. at 90°, cooled below 50°, and distilled in vacuo until dryness; the residue was taken up in C₆H₆ to give 38.8 g. MeC(OAc)(CN)CONH₂ (XI), m. 98-9° (AcOEt). A solution of 20 g. IIa in 200 ml. anhydrous C₅H₅N was treated at 0° with 20 g. ClSO₃H, the mixture kept overnight, with stirring, at room temperature and cooled to 0°, 42 g. NaHCO₃ added, stirring continued 3 hrs., the mixture filtered, the solution evaporated in vacuo to dryness, keeping the temperature below 30°, and the residue taken up in 100 ml. absolute EtOH to give 28.8 g. C₅H₅N salt of MeC(OSO₃H)(CN)CONH₂ (XII), m. 130-1° (MeOH). XII was dissolved in MeOH and treated with MeONa to give the corresponding Na salt, m. 185-7°. Through a solution of 20 g. IIa in 50 ml. MeOH, cooled at 5°, dry NH₃ gas was slowly passed during 12 hrs., the precipitated solid filtered off, the solution evapd. in vacuo to dryness, and the residue taken up in 20 ml. absolute EtOH, to give 9.5 g. MeC(NH₂)(CN)CONH₂ (XIII), m. 110-2° (C₂H₄Cl₂). The infrared spectra of III, IV, V, VI, VIII, IX, X, XI, XII, and XIII were given. The probable reaction mechanism as it results from the use of H¹⁴CN was discussed.

IT 89532-92-3, Lactamide, 2-cyano-, acetate (ester)
 (preparation of)
 RN 89532-92-3 HCAPLUS
 CN Lactamide, 2-cyano-, acetate (7CI) (CA INDEX NAME)



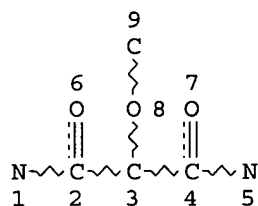
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L1 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L3 31 SEA FILE=REGISTRY SSS FUL L1
L6 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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L9 49 SEA FILE=REGISTRY ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN OR
OR DIBUTYLTIN OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR
PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
L11 643 SEA FILE=REGISTRY ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN
L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
L13 70 SEA FILE=HCAPLUS ABB=ON PLU=ON L8
L14 25437 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 OR TRIFLUOROACETIC(W) ANHYDR
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TRICHLORIDE OR PENTACHLORIDE?)

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OR ALCL3

L16 389244 SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEHYDRATION AGENTS"/CV OR
"DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR
DEHYDRAT? OR DRYING

L17 30094 SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEWIS ACIDS"/CV OR "CARBONYL
S (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/C
V OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV
) OR LEWIS(W)ACID

L20 4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L8 AND (L16 OR L14 OR L17 OR
L15)) NOT L12

L21 1744 SEA FILE=HCAPLUS ABB=ON PLU=ON CYANO(L)?ACETAMIDE?

L22 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (L21 AND L13) NOT L12

L23 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 OR L22

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L23 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:220131 HCAPLUS

DOCUMENT NUMBER: 142:298014

TITLE: Preparation of dibenzoazepinylmalonamides,
dibenzooxepinylmalonamides,
benzodiazepinylmalonamides, and related compounds as
γ-secretase inhibitors for treatment of
Alzheimer's disease.

INVENTOR(S): Flohr, Alexander; Galley, Guido; Jakob-Roetne, Roland;
Kitas, Eric Argirios; Peters, Jens-Uwe; Wostl,
Wolfgang

PATENT ASSIGNEE(S): Switz.

SOURCE: U.S. Pat. Appl. Publ., 59 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

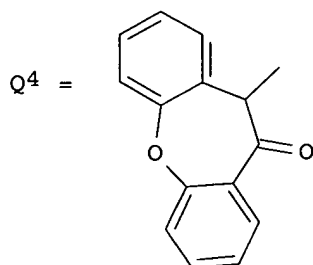
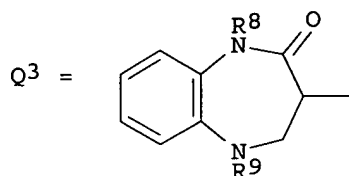
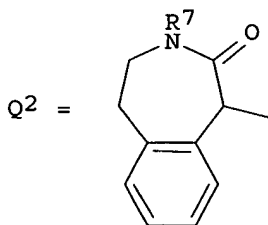
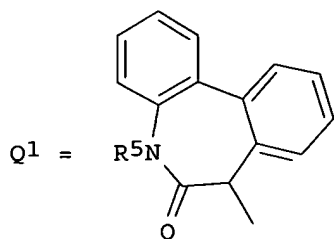
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005054633	A1	20050310	US 2004-933177	20040902
WO 2005023772	A1	20050317	WO 2004-EP9700	20040831
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: EP 2003-19683 A 20030909

OTHER SOURCE(S): MARPAT 142:298014

GI



AB Malonamides R1NHCOCR3R4CONHR2 [R1= Q1-Q4; R2 = alkyl, alkynyl, alkylthio, alkoxy(alkyl), halo(alkyl), etc.; R3, R4 = H, alkyl, alkoxy, Ph, halo; R5 = H, alkyl, trifluoromethyl(alkyl), cycloalkyl(alkyl); R6 = H, halo; R7 = H, alkyl; R8 = H, alkyl, alkynyl, trifluoromethyl(alkyl), cycloalkyl(alkyl), (halo-substituted) phenyl(alkyl); R9 = H, alkyl, CHO, alkylcarbonyl, F3CCO, (substituted) PhCO, etc.], were prepared Thus, 2-methyl-N-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonic acid (preparation given), cyclopropylmethylamine, and 2-(2-pyridon-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate (TPTU) were shaken together overnight in DMF to give N-cyclopropylmethyl-2-methyl-N'-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonamide. The latter inhibited γ -secretase with IC50 = 0.09 μ M.

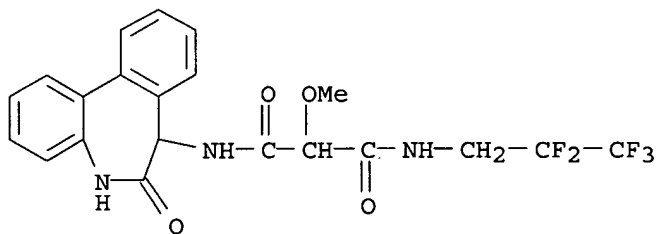
IT 847925-92-2P 847926-00-5P 847926-11-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of dibenzoazepinylmalonamides, dibenzoxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ -secretase inhibitors for treatment of Alzheimer's disease)

RN 847925-92-2 HCAPLUS

CN Propanediamide, N-(6,7-dihydro-6-oxo-5H-dibenz[b,d]azepin-7-yl)-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

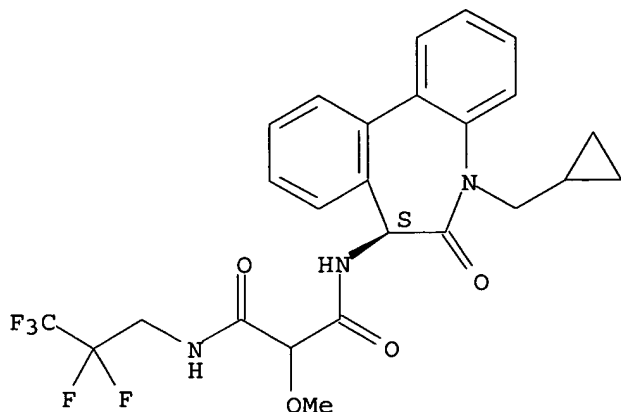


RN 847926-00-5 HCAPLUS

CN Propanediamide, N-[(7S)-5-(cyclopropylmethyl)-6,7-dihydro-6-oxo-5H-

dibenz[b,d]azepin-7-yl]-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI)
(CA INDEX NAME)

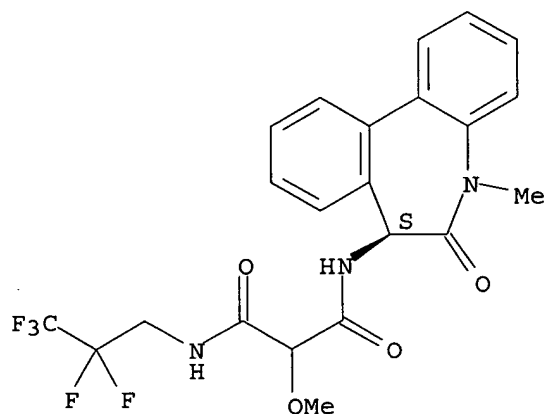
Absolute stereochemistry.



RN 847926-11-8 HCAPLUS

CN Propanediamide, N-[(7S)-6,7-dihydro-5-methyl-6-oxo-5H-dibenz[b,d]azepin-7-yl]-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 847927-37-1P

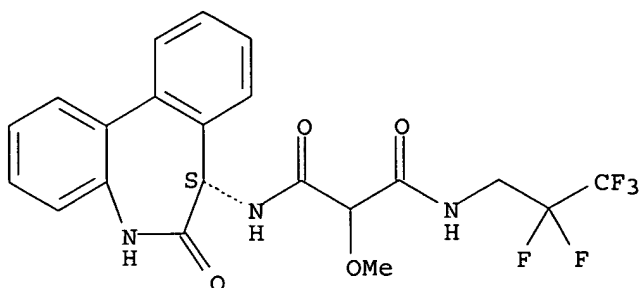
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dibenzoazepinylmalonamides, dibenzoxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ -secretase inhibitors for treatment of Alzheimer's disease)

RN 847927-37-1 HCAPLUS

CN Propanediamide, N-[(7S)-6,7-dihydro-6-oxo-5H-dibenz[b,d]azepin-7-yl]-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



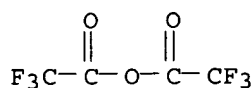
IT 407-25-0, **Trifluoroacetic anhydride**

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dibenzothiazepinylmalonamides, dibenzothiazepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ -secretase inhibitors for treatment of Alzheimer's disease)

RN 407-25-0 HCAPLUS

CN Acetic acid, trifluoro-, anhydride (6CI, 8CI, 9CI) (CA INDEX NAME)



L23 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:478964 HCAPLUS

DOCUMENT NUMBER: 113:78964

TITLE: Development of a new acyl anion equivalent for the preparation of masked activated esters, and their use to prepare a dipeptide

AUTHOR(S): Nemoto, Hisao; Kubota, Yasufumi; Yamamoto, Yoshinori

CORPORATE SOURCE: Fac. Sci., Tohoku Univ., Sendai, 980, Japan

SOURCE: Journal of Organic Chemistry (1990), 55(15), 4515-16

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:78964

AB New acyl anion equivs., the protected hydroxymalonitriles $\text{ROCH}(\text{CN})_2$ (I, R = CHMeOEt, SiMe₂CMe₃) have been developed as masked activated ester equivs. Alkylation or allylation of I (R = CHMeOEt) proceeded in high yields under mild basic or neutral conditions, resp. Treatment of the tosylamine 4-MeOC₆H₄CH₂NSO₂C₆H₄Me-4 with I (R = CHMeOEt) gave the dipeptide 4-MeOC₆H₄CH₂NR₂SO₂C₆H₄Me-4 (II, R₁ = CO-Gly-OMe, R₂ = CH₂OMe) via the α -amino acid II [R₁ = C(CN)₂OCHMeOEt, R₂ = H] having a masked activated functionality.

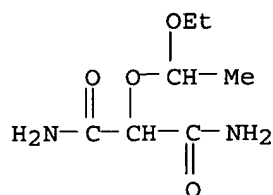
IT 128326-92-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and dehydration of, malononitrile derivative from)

RN 128326-92-1 HCAPLUS

CN Propanediamide, 2-(1-ethoxyethoxy)- (9CI) (CA INDEX NAME)



L23 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:437004 HCAPLUS

DOCUMENT NUMBER: 81:37004

TITLE: Light induced reactions of 4-n-butyl-1,2-diphenylpyrazolidine-3,5-dione (phenylbutazone) with nucleophilic agents

AUTHOR(S): Reisch, J.; Weidmann, K. G.; Triebe, J.

CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ. Muenster, Muenster/Westf., Fed. Rep. Ger.

SOURCE: Experientia (1974), 30(5), 451-2

CODEN: EXPEAM; ISSN: 0014-4754

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

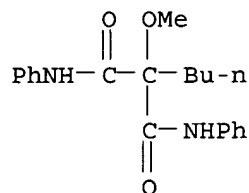
AB Uv irradiation of phenylbutazone (I) forms an aziridinone intermediate (II), which in the presence of MeOH or Me₂NH gives PhNHCOCBuRCONHPh (III; R = MeO, Me₂N). In H₂O solution II forms III (R = OH), which is **dehydrated** to PhNHCOC(:CHPr)CONHPr or decomp. to HCONHPh and PhNH₂.

IT 52884-93-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 52884-93-2 HCAPLUS

CN Propanediamide, 2-butyl-2-methoxy-N,N'-diphenyl- (9CI) (CA INDEX NAME)



L23 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:84132 HCAPLUS

DOCUMENT NUMBER: 78:84132

TITLE: Reaction of aliphatic isocyanides with chloroacetic anhydride and trifluoroacetic anhydride

AUTHOR(S): Krivinka, P.; Honzl, J.

CORPORATE SOURCE: Cesk. Akad. Ved, Prague, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1972), 37(12), 4035-40

CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB MeNC (I) and (ClCH₂CO)₂O (II) in CHCl₃ at 30° gave ClCH₂C(O)NMeCOCH₂Cl which was converted in aqueous tetrahydrofuran to ClCH₂C(OH)NMeCOCH₂Cl. Reaction of I and (F₃CCO)₂O (III) in CCl₄ and hydrolysis gave F₃CC(OH)NMe. Reaction of tert-BuNC (IV) and II in CHCl₃ and hydrolysis gave (tert-BuNHCO)₂C(CH₂Cl)OCOCH₂Cl (V). V kept in liquid NH₃ gave (tert-BuNHCO)₂C(CH₂Cl)OH. Reduction of V with activated Al in aqueous tetrahydrofuran gave (tert-BuNHCO)₂C(CH₂Cl)OAc. Reaction of III and IV in CCl₄ at 0° and decomposition with H₂O gave (tert-BuNHCO)₂C(OH)CF₃ (VI); decomposition with EtOH gave

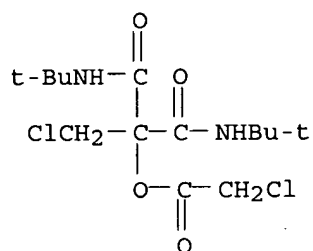
1-tert-butyl-3-hydroxy-3-(trifluoromethyl)-4-(tert-butylimino)-2-azetidinone (VII). Acetylation of VI (Ac₂O-pyridine) or VII [Pb(OAc)₄] gave (tert-BuNHCO)₂C(OAc)CF₃.

IT 39528-85-3P 39528-87-5P 39528-90-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

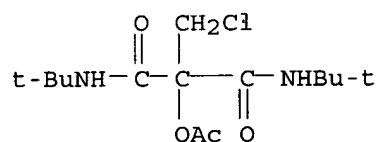
RN 39528-85-3 HCAPLUS

CN Acetic acid, chloro-, 1-(chloromethyl)-2-[(1,1-dimethylethyl)amino]-1-[[1,1-dimethylethyl)amino]carbonyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)



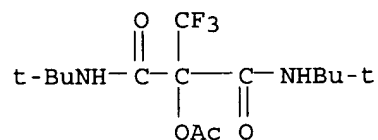
RN 39528-87-5 HCAPLUS

CN Propanediamide, 2-(acetyloxy)-2-(chloromethyl)-N,N'-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RN 39528-90-0 HCAPLUS

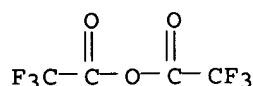
CN Propanediamide, 2-(acetyloxy)-N,N'-bis(1,1-dimethylethyl)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



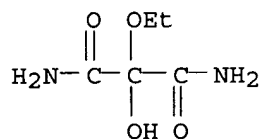
IT 407-25-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alkyl isocyanides)

RN 407-25-0 HCAPLUS
 CN Acetic acid, trifluoro-, anhydride (6CI, 8CI, 9CI) (CA INDEX NAME)



L23 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1964:432402 HCAPLUS
 DOCUMENT NUMBER: 61:32402
 ORIGINAL REFERENCE NO.: 61:5639f-h
 TITLE: Hydroxy-1,2,5-thiadiazoles. I. A novel route from potassium cyanide and sulfur dioxide
 AUTHOR(S): Ross, John M.; Smith, William C.
 CORPORATE SOURCE: E. I. du Pont de Nemours & Co. Inc., Wilmington, DE
 SOURCE: Journal of the American Chemical Society (1964), 86(14), 2861-8
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 61:32402
 GI For diagram(s), see printed CA Issue.
 AB 3-Cyano-4-hydroxy-1,2,5-thiadiazole (I) has been obtained from the reaction of KCN and SO₂ at 25-85° in the absence of hydroxylic solvents. The structure was elucidated by degradation to diethylaminoacetamide and to N-sulfamoyloxamic acid dipotassium salt, and by independent synthesis from isonitrosocyanoacetamide and S₂Cl₂. Various 3-hydroxy-1,2,5-thiadiazole derivs. were prepared including several K acid salts involving sym. Hbonding of the acidic 3-hydroxy proton.
 IT 89799-70-2, Tartronamide, 2-ethoxy- (preparation of)
 RN 89799-70-2 HCAPLUS
 CN Tartronamide, 2-ethoxy- (7CI) (CA INDEX NAME)



=> => d stat que 127 nos

L1 STR
 L3 31 SEA FILE=REGISTRY SSS FUL L1
 L6 STR
 L8 158 SEA FILE=REGISTRY SSS FUL L6
 L9 49 SEA FILE=REGISTRY ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN
 OR DIBUTYLTIN OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR
 PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
 L11 643 SEA FILE=REGISTRY ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN
 L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
 L14 25437 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 OR TRIFLUOROACETIC(W) ANHYDR
 IDE OR DIBUTYLTIN(W) OXIDE OR PHOSPHORUS(W) (OXYCHLORIDE? OR

TRICHLORIDE OR PENTACHLORIDE?)

L15 73122 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR ALUMINUM (W)CHLORIDE OR ALCL3

L16 389244 SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEHYDRATION AGENTS"/CV OR "DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR DEHYDRAT? OR DRYING

L17 30094 SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEWIS ACIDS"/CV OR "CARBONYL S (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/C V OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV) OR LEWIS(W)ACID

L20 4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L8 AND (L16 OR L14 OR L17 OR L15)) NOT L12

L26 15 SEA FILE=HCAPLUS ABB=ON PLU=ON "HILDBRAND STEFAN"/AU

L27 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L26 NOT (L12 OR L20)

=> d ibib abs 127 1-14

L27 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:221642 HCAPLUS

DOCUMENT NUMBER: 138:238184

TITLE: Amidation and hydrogenation method for producing beta-alanine amides from amines and cyanoacetate esters

INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**

PATENT ASSIGNEE(S): Lonza A.-G., Switz.

SOURCE: PCT Int. Appl., 21 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003022795	A1	20030320	WO 2002-EP9893	20020904
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1430018	A1	20040623	EP 2002-767473	20020904
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
JP 2005502697	T2	20050127	JP 2003-526873	20020904
US 2004220410	A1	20041104	US 2004-488692	20040305
PRIORITY APPLN. INFO.:			EP 2001-121342	A 20010906
			US 2001-332547P	P 20011126
			WO 2002-EP9893	W 20020904

OTHER SOURCE(S): CASREACT 138:238184; MARPAT 138:238184

AB β -Alanine amides R2(R1CH2)NCOCH2CH2NH2 [R1 = H, (un)substituted C1-6 alkyl; R2 = H; R1R2 = (CH2)n; n = 3, 4; e.g., carinine], used as an active ingredient having an antioxidative effect in medicaments and cosmetics (no data), are produced without using an amino protective group

by the amidation of the corresponding amine R2(R1CH2)NH (e.g., histamine) with a cyanoacetic ester R3O2CCH2CN (R3 = C1-10 alkyl; e.g., Et cyanoacetate) in order to form a cyanoacetamide R2(R1CH2)NCOCH2CN [e.g., 2-Cyano-N-[2-(1(3)H-imidazol-4-yl)ethyl]acetamide] and by subjecting the cyanoacetamide to catalytic hydrogenation.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:661387 HCAPLUS

DOCUMENT NUMBER: 135:211285

TITLE: Preparation of β -alaninamide dipeptides from N-unprotected amino acids or esters and cyanoacetic acid derivatives

INVENTOR(S): Hildbrand, Stefan; Ruppen, Thomas; Veghini, Dario

PATENT ASSIGNEE(S): Lonza A.-G., Switz.

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001064638	A1	20010907	WO 2001-EP2349	20010302
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US, US, US			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1259483	A1	20021127	EP 2001-936057	20010302
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004509834	T2	20040402	JP 2001-563481	20010302
US 2003105335	A1	20030605	US 2002-220608	20021121
US 6878829	B2	20050412		
US 2005192354	A1	20050901	US 2005-102828	20050411
PRIORITY APPLN. INFO.:			EP 2000-104643	A 20000303
			US 2001-271694P	P 20010228
			WO 2001-EP2349	W 20010302
			US 2002-220608	A3 20021121

OTHER SOURCE(S): CASREACT 135:211285; MARPAT 135:211285

AB The invention relates to β -alaninamides of general formula $H_2N(CH_2)_2C(O)N(R_2)CH(R_1)C(O)OR$ [R = H, a neg. charge compensated for by an equivalent of an inorg. or organic cation, or alkyl; R1 = H, (substituted) alkyl;

R2 = H, or R1 and R2, together, form a group of formula $-(CH_2)_n$; n = 3 or 4]. The β -alaninamides are produced without using an amino protective group by reacting the corresponding α -amino acid or the corresponding α -amino acid ester with a cyanoacetic acid to form a cyanoacetic acid amide and by a subsequent catalytic hydrogenation. The method is particularly suited for producing carnosine (β -alanyl-L-histidine), a naturally occurring dipeptide, which is used as a food additive having an antioxidant effect. Thus, cyanoacetic acid Et ester

was coupled to L-histidine and the resulting dipeptide hydrogenated using a rhodium catalyst to give L-carnosine (76% yield, 99.5% optical purity). Anserin (β -alanyl-3-methyl-L-histidine) was similarly prepared, in 45% yield, starting from 3-methyl-L-histidine and cyanoacetic acid Et ester.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:564992 HCAPLUS

DOCUMENT NUMBER: 135:122023

TITLE: Amidation and etherification method for producing N-alkoxy-N-alkylcarboxamides from carboxylate esters

INVENTOR(S): Hanselmann, Paul; Hildbrand, Stefan; Sterren, Etienne

PATENT ASSIGNEE(S): Lonza A.-G., Switz.

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001055096	A1	20010802	WO 2001-EP753	20010124
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US				
RW:				
GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1250316	A1	20021023	EP 2001-913765	20010124
EP 1250316	B1	20041229		
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520844	T2	20030708	JP 2001-555038	20010124
AT 286020	E	20050115	AT 2001-913765	20010124
US 2004030142	A1	20040212	US 2002-181420	20020724
US 6891049	B2	20050510		

PRIORITY APPLN. INFO.:

EP 2000-101391 A 20000125
US 2000-203906P P 20000512
WO 2001-EP753 W 20010124

OTHER SOURCE(S): CASREACT 135:122023; MARPAT 135:122023

AB N-alkoxy-N-alkylcarboxamides R1CON(R2)(OR2) (R1 = C1-10 alkyl, cycloalkyl, cycloalkenyl, C2-10 alkenyl, aryl, arylalkyl, heteroaryl, heteroarylalkyl, heterocyclyl; R2 = C1-6 alkyl) (e.g., N-methoxy-N-methyl-2-furancarboxamide) are prepared in high yield and selectivity by the amidation of carboxylate esters R1COOR3 (R3 = C1-6 alkyl, 4-nitrophenyl, 2,4-dinitrophenyl, succinimido, benzotriazole-1-yl) (e.g., Me 2-furancarboxylate) with hydroxylamine, a hydroxylamine derivative, or with a hydroxylammonium salt (e.g., hydroxylammonium sulfate), and the reaction product is alkylated and etherified with R2X (X = halogen) (e.g., chloromethane) in the presence of a phase-transfer catalyst (e.g., tetrabutylammonium bromide).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:167957 HCAPLUS
 DOCUMENT NUMBER: 134:207549
 TITLE: Oxidative method and catalysts for producing
 cyanoacetate esters from 3-(alkoxy)propionitriles
 INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**
 PATENT ASSIGNEE(S): Lonza A.-G., Switz.
 SOURCE: PCT Int. Appl., 14 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016092	A1	20010308	WO 2000-EP8397	20000829
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1208081	A1	20020529	EP 2000-964050	20000829
EP 1208081	B1	20040414		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
JP 2003532628	T2	20031105	JP 2001-519662	20000829
AT 264296	E	20040415	AT 2000-964050	20000829
ES 2219396	T3	20041201	ES 2000-964050	20000829
TW 572875	B	20040121	TW 2000-89127179	20001219
US 6700010	B1	20040302	US 2002-69579	20020712
HK 1048107	A1	20050527	HK 2003-100196	20030108
PRIORITY APPLN. INFO.:			EP 1999-117033	A 19990830
			US 2000-185372P	P 20000228
			WO 2000-EP8397	W 20000829

OTHER SOURCE(S): CASREACT 134:207549; MARPAT 134:207549

AB Cyanoacetate esters NCCH₂CO₂R [R = (un)substituted (un)branched C1-8 alkyl, arylalkyl] (e.g., Me 2-cyanoacetate) are prepared in high yield and selectivity by the oxidation of 3-(alkoxy)propionitriles RO(CH₂)₂CN (e.g., 3-methoxypropionitrile) in the presence of a catalyst based on lead or on one of the transition metals (e.g., cobalt diacetate tetrahydrate) using oxygen or an oxygen-forming reagent (e.g., N-hydroxyphthalimide).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:573541 HCAPLUS
 DOCUMENT NUMBER: 133:164469
 TITLE: Preparation of cyanoacetate esters
 INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**
 PATENT ASSIGNEE(S): Lonza A.-G., Switz.
 SOURCE: Eur. Pat. Appl., 5 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1028105	A1	20000816	EP 2000-102087	20000203
EP 1028105	B1	20040421		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
IL 134110	A1	20041215	IL 2000-134110	20000118
TW 526186	B	20030401	TW 2000-89100864	20000120
KR 2000057793	A	20000925	KR 2000-3077	20000122
CN 1266845	A	20000920	CN 2000-101944	20000131
CA 2297636	AA	20000809	CA 2000-2297636	20000203
AT 264836	E	20040515	AT 2000-102087	20000203
PT 1028105	T	20040930	PT 2000-102087	20000203
ES 2220265	T3	20041216	ES 2000-102087	20000203
JP 2000229930	A2	20000822	JP 2000-27076	20000204
NO 2000000625	A	20000810	NO 2000-625	20000208
US 6239307	B1	20010529	US 2000-500634	20000209
HK 1030205	A1	20041119	HK 2001-101240	20010221
PRIORITY APPLN. INFO.:			EP 1999-102286	A 19990209
			US 1999-145997P	P 19990729

OTHER SOURCE(S): MARPAT 133:164469

AB In the title process, in which aqueous NCCH₂CO₂Na solns. can be esterified directly, the alkali cyanoacetate solution is treated with alkyl, alkenyl, or aryl halides in 2-phase H₂O-organic systems in the presence of phase-transfer catalysts. Adding 0.20 mol MeCl to a mixture of 0.02 mol NCCH₂CO₂H, 0.02 mol NaOH, 2.0 mmol Bu₄N⁺ Br⁻, and 15 mL 2:1 tert-BuOMe-H₂O, heating over 30 min to 100°, and holding at 100°/10 bar for 3.5 h gave 68% NCCH₂CO₂Me.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:501822 HCAPLUS

DOCUMENT NUMBER: 133:89232

TITLE: Preparation of malonic esters

INVENTOR(S): Hildbrand, Stefan; Hanselmann, Paul

PATENT ASSIGNEE(S): Lonza A.-G., Switz.

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000204061	A2	20000725	JP 2000-1898	20000107
EP 1026148	A1	20000809	EP 2000-100310	20000107
EP 1026148	B1	20030507		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 239692	E	20030515	AT 2000-100310	20000107
PT 1026148	T	20030930	PT 2000-100310	20000107
SK 283638	B6	20031104	SK 2000-24	20000107
ES 2199100	T3	20040216	ES 2000-100310	20000107
NO 2000000109	A	20000712	NO 2000-109	20000110
NO 314757	B1	20030519		
KR 2000053438	A	20000825	KR 2000-896	20000110

US 6350898 B1 20020226 US 2000-480165 20000110
 CN 1263885 A 20000823 CN 2000-101055 20000111
 PRIORITY APPLN. INFO.: EP 1999-100411 A 19990111
 OTHER SOURCE(S): CASREACT 133:89232; MARPAT 133:89232
 AB Title compds. CH₂(CO₂R)₂ (R = alkyl, alkenyl, arylalkyl) are prepared by reaction of alkali salts of malonic acid with RX (X = halo) in water in the presence of phase transfer catalysts. Thus, reaction of disodium malonate with MeCl in H₂O in the presence of Bu₄NBr at 100° for 3 h gave 48% di-Me malonate.

L27 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:384137 HCAPLUS
 DOCUMENT NUMBER: 133:32023
 TITLE: Manufacture of hydroxamic acid esters in one-pot amidation-alkylation of corresponding esters
 INVENTOR(S): Hanselmann, Paul; Hildbrand, Stefan
 PATENT ASSIGNEE(S): Lonza AG, Switz.
 SOURCE: PCT Int. Appl., 15 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000032564	A1	20000608	WO 1999-EP9121	19991125
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: EP 1998-122927 A 19981203
 OTHER SOURCE(S): MARPAT 133:32023

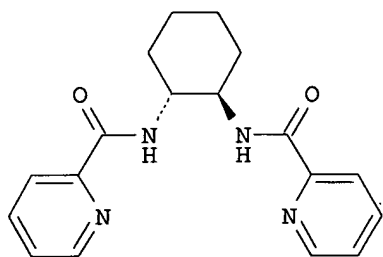
AB Hydroxamic acid esters are manufactured in a one-pot process involving aqueous reaction of a corresponding ester with a hydroxylammonium salt (typically hydroxylamine hydrochloride or hydroxylamine sulfate) in the presence of strong base, followed by base-catalyzed alkylation with a dialkyl sulfate or an alkyl chloride. The intermediate hydroxy amides are not isolated; the product O-alkyl hydroxamic esters is prepared in high yield with minimal content of N,O-dialkylated byproducts. The hydroxamic acid esters have the general formula R₁R₂C=C(R₃)-C(:O)-NH-OR, which are derived from the corresponding esters, of general formula R₁R₂C=C(R₃)-C(:O)-O-R' (R = C1-6-alkyl; R₁-3 = H or C1-4-alkyl; and R' = C1-6-alkyl). Alkylation is carried out using, as alkylating agents, a dialkyl sulfate, (RO)₂SO₂, or an alkyl chloride, RCl (R = C1-6-alkyl). The hydroxamic acid ester are suitable as blocking agents for isocyanates.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

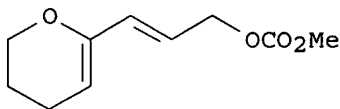
L27 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:680946 HCAPLUS
 DOCUMENT NUMBER: 132:78124
 TITLE: Regio- and enantioselective molybdenum-catalyzed alkylations of polyenyl esters
 AUTHOR(S): Trost, Barry M.; Hildbrand, Stefan; Dogra,

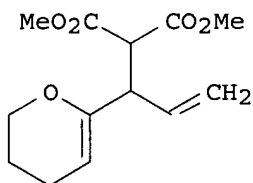
Kalindi
 CORPORATE SOURCE: Department of Chemistry, Stanford University,
 Stanford, CA, 94305-5080, USA
 SOURCE: Journal of the American Chemical Society (1999),
 121(44), 10416-10417
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 132:78124
 GI



II



III



IV

AB The title reaction was examined using $(\text{EtCN})_3\text{Mo}(\text{CO})_3$ (I) as catalyst and several diamine ligands. Thus, reacting $\text{PhCH:CHCH:CHCH}_2\text{OCO}_2\text{Me}$ with $(\text{MeO}_2\text{C})_2\text{CH}$ using I and diamine II gave $(\text{MeO}_2\text{C})_2\text{CC}(\text{CH:CH}_2)\text{CH:CHPh}$ in 98% ee. Polyenyl carbonate III gave diester IV in 96% ee after 1.5 h.
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1998:272282 HCAPLUS
 DOCUMENT NUMBER: 129:51267
 TITLE: Inhibition of DNA polymerase reactions by pyrimidine nucleotide analogs lacking the 2-keto group
 AUTHOR(S): Guo, Mao-Jun; **Hildbrand, Stefan**; Leumann, Christian J.; McLaughlin, Larry W.; Waring, Michael J.
 CORPORATE SOURCE: Department of Pharmacology, University of Cambridge, Cambridge, CB2 1QJ, UK
 SOURCE: Nucleic Acids Research (1998), 26(8), 1863-1869
 CODEN: NARHAD; ISSN: 0305-1048
 PUBLISHER: Oxford University Press
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB To investigate the influence of the pyrimidine 2-keto group on selection

of nucleotides for incorporation into DNA by polymerases, we have prepared two C nucleoside triphosphates that are analogs of dCTP and dTTP, namely 2-amino-5-(2'-deoxy- β -D-ribofuranosyl)pyridine-5'-triphosphate (d*CTP) and 5-(2'-deoxy- β -D-ribofuranosyl)-3-methyl-2-pyridone-5'-triphosphate (d*TTP) resp. Both proved strongly inhibitory to PCR catalyzed by Taq polymerase; d*TTP rather more so than d*CTP. In primer extension expts. conducted with either Taq polymerase or the Klenow fragment of Escherichia coli DNA polymerase I, both nucleotides failed to substitute for their natural pyrimidine counterparts. Neither derivative was incorporated as a chain terminator. Their capacity to inhibit DNA polymerase activity may well result from incompatibility with the correctly folded form of the polymerase enzyme needed to stabilize the transition state and catalyze phosphodiester bond formation.

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:740245 HCAPLUS

DOCUMENT NUMBER: 127:346619

TITLE: Preparation of modified cytidine-containing oligodeoxyribonucleotide triplexes

INVENTOR(S): Leumann, Christian; **Hildebrand, Stefan**

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Leumann, Christian; Hildebrand, Stefan

SOURCE: PCT Int. Appl., 72 pp.

CODEN: PIXXD2

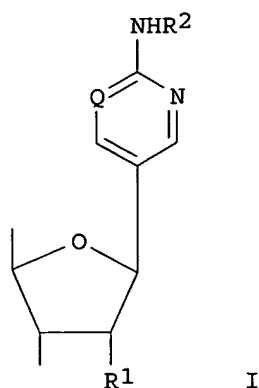
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9741140	A1	19971106	WO 1997-EP1856	19970414
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9726968	A1	19971119	AU 1997-26968	19970414
PRIORITY APPLN. INFO.:			CH 1996-1059	A 19960426
			WO 1997-EP1856	W 19970414
OTHER SOURCE(S):		MARPAT 127:346619		
GI				



AB Oligodeoxyribonucleotide in which at least one cytidine building block is replaced with an analogous building block I [Q = N, CR; R = H, alkyl; R1 = H, (un)substituted alkyl, alkoxy, oxymethyl-heterocycle; R2 = H, alkyl, aminoalkyl, alkylamino, alkoxyalkyl] in which the cytidine residue is replaced with a C-bonded aminopyridyl or aminopyrimidyl were prepared. Affinity and interaction of these oligodeoxyribonucleotides with DNA duplexes is reported. Thermal stability and hyperchromicity of these DNA triplexes are reported.

L27 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:347278 HCAPLUS

DOCUMENT NUMBER: 127:66082

TITLE: 5-Substituted 2-Aminopyridine C-Nucleosides as Protonated Cytidine Equivalents: Increasing Efficiency and Specificity in DNA Triple-Helix Formation

AUTHOR(S): Hildbrand, Stefan; Blaser, Adrian; Parel, Serge P.; Leumann, Christian J.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Bern, Bern, CH-3012, Switz.

SOURCE: Journal of the American Chemical Society (1997), 119(24), 5499-5511

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The easily accessible C-nucleoside 2-amino-5-(2'-deoxy-β-D-ribofuranosyl)pyridine (P) and its 3-Me (X) and 2'-O-Me (Y) derivs. were synthesized and incorporated as protonated cytidine equivalent in homopyrimidine oligodeoxyribonucleotides. T_m measurements indicate that oligodeoxyribonucleotides containing P or X have a higher affinity to double-stranded DNA over the pH range of 6-8 than 5-methylcytidine (Z) containing oligodeoxyribonucleotides. This increase in stability is most pronounced above pH 7.0. The average increase in T_m/modification for the dissociation of oligodeoxyribonucleotide d(TTTTXXTXXTXXTXXT) from a 21-mer target duplex at pH 7.5 is 2.3 °C relative to oligodeoxyribonucleotide d(TTTTZZTZZTZZTZZT). The pH dependence and sequence composition effects are much less pronounced for X (and also P) containing

oligodeoxyribonucleotides than for Z containing ones. While oligodeoxyribonucleotide d(TTTZZZZTTTZZTTT) has already no longer any affinity to the target duplex above pH 6.5, oligodeoxyribonucleotide d(TTTXXXXTTTXXTTT) displays preserved binding with a T_m of 32.5 °C

at pH 7.0 and even binds with a T_m of 23.3 °C at pH 8.0. The average decrease in T_m /modification for oligodeoxyribonucleotide d(TTTTTYTYTYTYTYT) at pH 6.5 is 6.7 °C relative to the Z containing oligodeoxyribonucleotide. DNase I footprint titration expts. indicate that d(TTTTXXTXTXTXTX) binds not only five times stronger to a 229 base pair DNA fragment than d(TTTTZZTZTZTZTZ) but also with higher selectivity.

Thus the new bases P and X show Hoogsteen specific pairing behavior.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:595218 HCAPLUS

DOCUMENT NUMBER: 126:8456

TITLE: Enhancing DNA triple helix stability at neutral pH by the use of oligonucleotides containing a more basic deoxycytidine analog.

AUTHOR(S): Hildbrand, Stefan; Leumann, Christian

CORPORATE SOURCE: Inst. organische, Chemie der Univ., Bern, CH-3012, Switz.

SOURCE: Angewandte Chemie, International Edition in English (1996), 35(17), 1968-1970

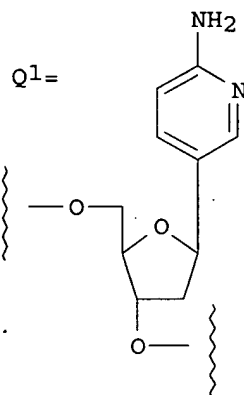
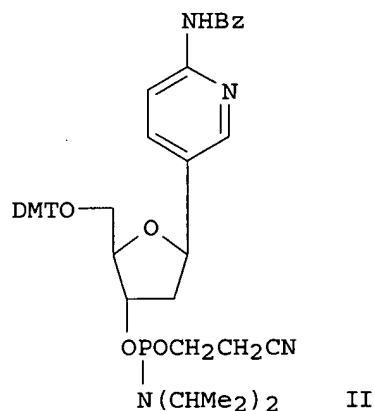
CODEN: ACIEAY; ISSN: 0570-0833

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB 5'-D(TTTTXXTXTXTXTX) (X = Q1), prepared using phosphoramidite (I) (preparation given) showed a dramatic increase in T_m for third-strand dissociation from a 21-mer duplex. Due to enhanced basicity, Q1 is an excellent substitute for cytidine in DNA duplex recognition at physiol. pH through the py:pu-py motif. The lack of the 2-oxo function does not perturb third-strand binding in the major groove of DNA.

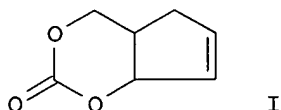
L27 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:322759 HCAPLUS

DOCUMENT NUMBER: 125:143183

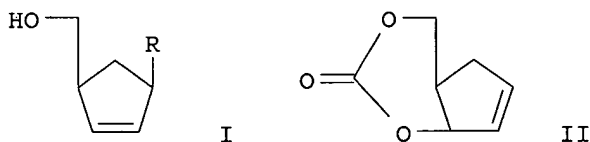
TITLE: Synthesis of carbocyclic C-nucleosides containing non-natural pyrimidine bases

AUTHOR(S): **Hildbrand, Stefan; Leumann, Christian; Scheffold, Rolf**
 CORPORATE SOURCE: Inst. organische Chemie, Univ. Bern, Bern, CH-3012, Switz.
 SOURCE: Helvetica Chimica Acta (1996), 79(3), 702-709
 CODEN: HCACAV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



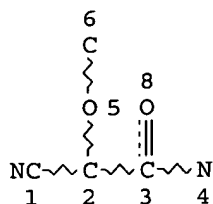
AB A series of carbocyclic C-nucleosides with a cis-4'-(hydroxymethyl)cyclopent-2'-enyl sugar moiety and unnatural pyrimidine bases were synthesized in racemic form in 2 steps starting from the easily accessible carbonate I.

L27 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:53074 HCAPLUS
 DOCUMENT NUMBER: 122:10439
 TITLE: A short synthesis of (-)-carbovir
 AUTHOR(S): **Hildbrand, Stefan; Troxler, Thomas; Scheffold, Rolf**
 CORPORATE SOURCE: Inst. Organ. Chem., Univ. Bern, Bern, CH-3012, Switz.
 SOURCE: Helvetica Chimica Acta (1994), 77(5), 1236-40
 CODEN: HCACAV; ISSN: 0018-019X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Carbovir (-)-I (R = guanine) was synthesized via the cyclic carbonate II in four steps starting from enantiomerically enriched (cyclopentenyl)methanol (-)-I (R = H).

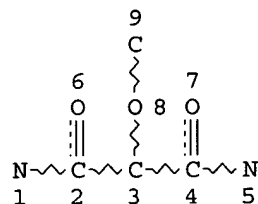
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 L1 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

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 NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
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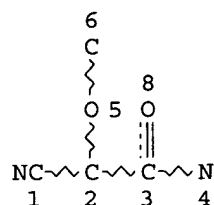
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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 L9 49 SEA FILE=REGISTRY ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN
 OR DIBUTYLTIN OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR
 PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
 L11 643 SEA FILE=REGISTRY ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN
 L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
 L13 70 SEA FILE=HCAPLUS ABB=ON PLU=ON L8
 L14 25437 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 OR TRIFLUOROACETIC (W) ANHYDR
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 TRICHLORIDE OR PENTACHLORIDE?)
 L15 73122 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR ALUMINUM (W) CHLORIDE
 OR ALCL3
 L16 389244 SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEHYDRATION AGENTS"/CV OR
 "DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR
 DEHYDRAT? OR DRYING
 L17 30094 SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEWIS ACIDS"/CV OR "CARBONYL
 S (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/C
 V OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV
) OR LEWIS (W) ACID
 L20 4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L8 AND (L16 OR L14 OR L17 OR
 L15)) NOT L12

L24 62 SEA FILE=HCAPLUS ABB=ON PLU=ON ("BARTEK J"/AU OR "BARTEK J P"/AU) OR "BARTEK JOHANNES"/AU
 L25 222 SEA FILE=HCAPLUS ABB=ON PLU=ON ("FUCHS R"/AU OR "FUCHS R A"/AU OR "FUCHS R E M"/AU OR "FUCHS R F"/AU OR "FUCHS R J"/AU OR "FUCHS R K"/AU OR "FUCHS R L"/AU OR "FUCHS R M"/AU OR "FUCHS R P"/AU OR "FUCHS R P P"/AU OR "FUCHS R R"/AU OR "FUCHS R WAYNE"/AU) OR "FUCHS RUDOLF"/AU
 L26 15 SEA FILE=HCAPLUS ABB=ON PLU=ON "HILDBRAND STEFAN"/AU
 L27 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L26 NOT (L12 OR L20)
 L29 0 SEA FILE=HCAPLUS ABB=ON PLU=ON ((L24 OR L25) AND L13) NOT (L12 OR L20 OR L27)

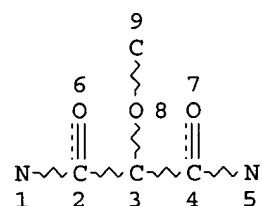
=> => d stat que l34
 L1 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
 L3 31 SEA FILE=REGISTRY SSS FUL L1
 L6 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
 L8 158 SEA FILE=REGISTRY SSS FUL L6
 L9 49 SEA FILE=REGISTRY ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN OR DIBUTYLTIN OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
 L11 643 SEA FILE=REGISTRY ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN
 L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
 L14 25437 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 OR TRIFLUOROACETIC (W) ANHYDR

IDE OR DIBUTYLTIN(W) OXIDE OR PHOSPHORUS(W) (OXYCHLORIDE? OR TRICHLORIDE OR PENTACHLORIDE?)

L15 73122 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR ALUMINUM (W)CHLORIDE OR ALCL3

L16 389244 SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEHYDRATION AGENTS"/CV OR "DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR DEHYDRAT? OR DRYING

L17 30094 SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEWIS ACIDS"/CV OR "CARBONYL S (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/C V OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV) OR LEWIS(W)ACID

L20 4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L8 AND (L16 OR L14 OR L17 OR L15)) NOT L12

L26 15 SEA FILE=HCAPLUS ABB=ON PLU=ON "HILDBRAND STEFAN"/AU

L27 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L26 NOT (L12 OR L20)

L30 5603 SEA FILE=HCAPLUS ABB=ON PLU=ON (L16 OR L14) AND (L17 OR L15)

L31 1285 SEA FILE=REGISTRY ABB=ON PLU=ON MALONAMIDE?

L32 3721 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 OR ?MALOMAMIDE?

L33 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND L30

L34 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 NOT (L12 OR L20 OR L27)

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L34 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:203862 HCAPLUS

DOCUMENT NUMBER: 142:429941

TITLE: Process for preparation of malononitrile

INVENTOR(S): Wu, Zongtao; Wang, Xinggen; Zhou, Jian; Wu, Kai

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 4 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CN 1451649	A	20031029	CN 2003-113472	20030512
PRIORITY APPLN. INFO.:			CN 2003-113472	20030512

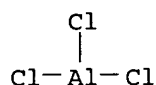
OTHER SOURCE(S): CASREACT 142:429941

AB This invention pertains to a method for producing malononitrile by **dehydration** of cyanoacetamide in 1,1,2-trichloroethane in the presence of **AlCl₃**-diethylamine HCl- pyridine (1:1.2-1.8:0.5-1.5) composite catalyst and POCl₃ **dehydration** agent at 50-114 °C for 0.5-5 h under collecting product and absorbing HCl gas with adsorption tower.

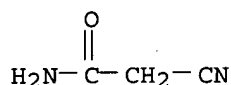
IT **7446-70-0, Aluminum chloride**, uses
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of malononitrile by **dehydration** of cyanoacetamide)

RN 7446-70-0 HCAPLUS

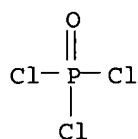
CN Aluminum chloride (AlCl₃) (9CI) (CA INDEX NAME)



IT 107-91-5, Cyanoacetamide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of malononitrile by **dehydration** of cyanoacetamide)
 RN 107-91-5 HCAPLUS
 CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 10025-87-3, Phosphorus oxychloride
 RL: RGT (Reagent); RACT (Reactant or reagent)
 (preparation of malononitrile by **dehydration** of cyanoacetamide)
 RN 10025-87-3 HCAPLUS
 CN Phosphoric trichloride (9CI) (CA INDEX NAME)



L34 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:220485 HCAPLUS
 DOCUMENT NUMBER: 134:237219
 TITLE: Process for preparing propanedinitrile
 INVENTOR(S): Cao, Jianbing
 PATENT ASSIGNEE(S): Zhennan Chemical Plant, Peop. Rep. China
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 8 pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CN 1264701	A	20000830	CN 1999-100873	19990224
PRIORITY APPLN. INFO.:			CN 1999-100873	19990224

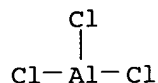
OTHER SOURCE(S): CASREACT 134:237219

AB The process comprises aminating Me cyanoacetate with NH₃ in methanol at (-5)-40°, **drying** at 50-110°, **dehydrating** with POCl₃ in dichloroethane in the presence of catalyst at 40-90°, separating, and distilling at 130-135° and 1.8-2.2 kPa. The catalyst is composed of diethylamine HCl 1, anhydrous pyridine 1, and anhydrous AlCl₃ 1 part.

IT 7446-70-0, Aluminum chloride (AlCl₃)
), uses
 RL: CAT (Catalyst use); USES (Uses)

(process for preparing propanedinitrile)

RN 7446-70-0 HCAPLUS

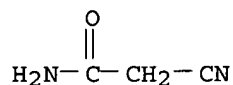
CN Aluminum chloride (AlCl₃) (9CI) (CA INDEX NAME)

IT 107-91-5P, Cyanoacetamide

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparing propanedinitrile)

RN 107-91-5 HCAPLUS

CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)

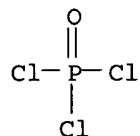


IT 10025-87-3, Phosphorus oxychloride

RL: RCT (Reactant); RACT (Reactant or reagent)
(process for preparing propanedinitrile)

RN 10025-87-3 HCAPLUS

CN Phosphoric trichloride (9CI) (CA INDEX NAME)



L34 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:862111 HCAPLUS

DOCUMENT NUMBER: 133:362558

TITLE: Process for preparing high-purity malononitrile

INVENTOR(S): Wu, Zongtao; Wang, Xinggen; Zhou, Jian

PATENT ASSIGNEE(S): Tongyuan Fine Chemical Plant, Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 6 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

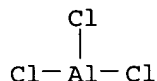
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CN 1250773	A	20000419	CN 1998-111530	19981009
CN 1086691	B	20020626		
PRIORITY APPLN. INFO.:			CN 1998-111530	19981009
OTHER SOURCE(S):		CASREACT 133:362558		

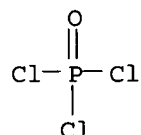
AB The process comprises reaction of Me cyanoacetate with NH₃ at 10-60° to obtain cyanoacetamide, **dehydration** with POCl₃ in organic solvent in the presence of catalyst at 60-90° for 4-12 h to

obtain crude malonitrile; recrystg. in anhydrous ethanol, and distilling at 109-120° and 16-22 mmHg. The catalyst is composed of diethylamine hydrochloride 1.2-1.8, AlCl₃ 1.0, and pyridine 0.5-1.5 part. The ratio of cyanoacetamide-POCl₃-organic solvent-catalyst is 1:1.0-1.4:1.7-6.04:0.01-0.10. The organic solvent is methanol or ethanol.

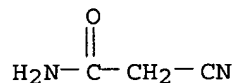
IT 7446-70-0, Aluminum trichloride, uses
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of high-purity malononitrile)
 RN 7446-70-0 HCAPLUS
 CN Aluminum chloride (AlCl₃) (9CI) (CA INDEX NAME)



IT 10025-87-3, Phosphoryl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of high-purity malononitrile)
 RN 10025-87-3 HCAPLUS
 CN Phosphoric trichloride (9CI) (CA INDEX NAME)



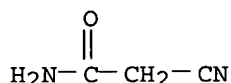
IT 107-91-5P, Cyanoacetamide
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of high-purity malononitrile)
 RN 107-91-5 HCAPLUS
 CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



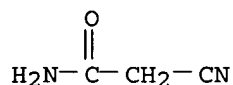
L34 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:716299 HCAPLUS
 DOCUMENT NUMBER: 125:328111
 TITLE: Process and phosphorous-compound catalysts for the
 preparation of nitriles from carboxamides
 INVENTOR(S): Hermeling, Dieter; Siegel, Haro
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: Ger. Offen., 4 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 DE 19515989 A1 19961107 DE 1995-19515989 19950502
 PRIORITY APPLN. INFO.: DE 1995-19515989 19950502
 OTHER SOURCE(S): CASREACT 125:328111; MARPAT 125:328111
 AB Nitriles R1CN [R1 = (un)substituted alkyl, (un)substituted cycloalkyl,
 (un)substituted Ph] (e.g., 1,8-dicyanooctane) are prepared in high yield and
 purity by the **dehydration** of carboxamides R1CONH2 (e.g.,
 decanedicarboxylic acid diamide) at 20-150°/0.01-5 bar in a
 suspension in an inert solvent (e.g., PhMe) in the presence of a P compound
 catalyst (e.g., Ph3P:O) or their adducts with acids (e.g., phosgene) or
 Lewis acids.
 IT 107-91-5, Cyanoacetamide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process and phosphorous-compound catalysts for the preparation of nitriles
 from carboxamides)
 RN 107-91-5 HCAPLUS
 CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)

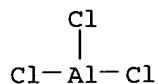


L34 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1978:546397 HCAPLUS
 DOCUMENT NUMBER: 89:146397
 TITLE: Studies on the optimization of cyanoacetamide to
 malononitrile **dehydration**
 AUTHOR(S): Malinowski, Romuald; Legocki, Jan
 CORPORATE SOURCE: Pol.
 SOURCE: Organika (1977) 53-61
 CODEN: ORGAD2; ISSN: 0137-9933
 DOCUMENT TYPE: Journal
 LANGUAGE: Polish
 AB The **dehydration** of cyanoacetamide to CH2(CN)2 with POCl3 in the
 presence of small amts. of CaCl2 or **AlCl3**, to prevent formation
 of polymeric metaphosphoric acid, was studied. Thus, cyanoacetamide (1
 mol) and 0.12 mol CaCl2 or 0.05 mol **AlCl3** are added to 168-210 g
 EtCl. The mixture is stirred and then 0.7 mol POCl3 is gradually added.
 The reaction mixture is heated to 90° for 6-7 h, then cooled to
 20°. The filtrate is distilled at 10-15 mm Hg to give a yield of
 88.4%.
 IT 107-91-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**dehydration** of)
 RN 107-91-5 HCAPLUS
 CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 7446-70-0, uses and miscellaneous
 RL: USES (Uses)
 (**dehydration** of cyanoacetamide in presence of)
 RN 7446-70-0 HCAPLUS

CN Aluminum chloride (AlCl3) (9CI) (CA INDEX NAME)



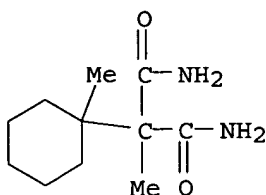
L34 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1958:11281 HCAPLUS
 DOCUMENT NUMBER: 52:11281
 ORIGINAL REFERENCE NO.: 52:2062c-f
 TITLE: Substituted methylmalononitriles
 INVENTOR(S): Westfahl, Jerome C.
 PATENT ASSIGNEE(S): B. F. Goodrich Co.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2802019		19570806	US	

AB Derivs. of methylmalononitrile were prepared by the addition of aliphatic and alicyclic hydrocarbons possessing a tertiary C atom to 1,1-dicyanoethene (I). To a mixture of 133.3 parts anhydrous sublimed **AlCl3** and 250 ml. dry (Cl2CH)2 (II) was added in 47 min. with stirring at 40° a solution of I 41.5, isopentane (dried with P2O5) 36.1 parts, and 150 ml. II. The mixture was stirred 30 min. without heating and then hydrolyzed by pouring into 1 l. crushed ice containing 50 ml. concentrated HCl. The usual processing gave 2,2-dicyano-3,3-dimethylpentane, m. 44.4° (MeOH). Similarly was prepared 1-(1-methylcyclohexyl)-1-methylmalononitrile (III), b. 99-9.5°. Hydrolysis of 4.9 parts III with 20 ml. 95% H2SO4 at 90° for 5 min., pouring into 200 ml. cold H2O and washing the precipitate with 5% NaOH, and then H2O followed by **drying** gave 1-(1-methylcyclohexyl)-1-methylcyanoacetamide, m. 154.3-55° (C6H6-C6H14). III 10 and KOH 30 parts in H2O 30 and EtOH 125 ml. were refluxed 263 hrs. More H2O was then added and the EtOH distilled. Acidification of the distillate to Congo red, shaking with Et2O and filtration gave (1-methylcyclohexyl)methylmalonamide, m. 239° (EtOH). The above H2O and Et2O layers were separated and the aqueous layer extracted with Et2O. This extract was combined with the Et2O layer and extracted with aqueous NaHCO3. The resulting H2O layer was separated and acidified to give (1-methylcyclohexyl)methylcyanoacetic acid (IV), m. 103.5-4.5° (C6H6-C6H14). Heating IV gave 1-(1-methylcyclohexyl)propionitrile (V), b. 220-7°, n25D 1.4631. Heating V with 95% H2SO4 gave 1-(1-methylcyclohexyl)propionamide, m. 108-8.5° (C6H6-C6H14).

IT **99991-57-8**, Cyclohexanemalonamide, α,1-dimethyl- (preparation of)
 RN 99991-57-8 HCAPLUS
 CN Cyclohexanemalonamide, α,1-dimethyl- (6CI) (CA INDEX NAME)



L34 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1949:11226 HCAPLUS

DOCUMENT NUMBER: 43:11226

ORIGINAL REFERENCE NO.: 43:2271e-i,2272a-i,2273a-i,2274a-b

TITLE: Biosynthesis of penicillins. III. Preparation and

evaluation of precursors for new penicillins

AUTHOR(S): Behrens, Otto K.; Corse, Joseph; Huff, Dorothea E.;
Jones, Reuben G.; Soper, Quentin F.; Whitehead,
Calvert W.SOURCE: Journal of Biological Chemistry (1948), 175, 771-92
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Methods are described for evaluation of compds. as precursors for new penicillins: (a) The ratio of units in the test container to units in control. Comparable results were obtained from *P. notatum* NRRL 1976 and *P. chrysogenum* Q-176. Stimulation may be interpreted as utilization of compound as a precursor. Lack of stimulation does not necessarily mean lack of utilization. (b) The ratio of antibacterial activity for *Bacillus subtilis* to that for *Staphylococcus aureus* compared with the same ratio using pure benzylpenicillin, which is defined as 1.0. (c) The relative position of the active portion in an adsorption column indicates a new penicillin. Culturing with N-2-hydroxyethyl- α -(allylmercapto)acetamide (I) deposited a new penicillin in a column. (d) The Craig method was used to determine the distribution coeffs. of the penicillins (C.A. 41, 6672i) formed between acid and ether. The penicillin formed using p-HSC₆H₄SCH₂CO₂H showed coeffs. and activities different from the controls while the activities and coeffs. with p-H₂O₃AsC₆H₄NHSO₂C₆H₄SCH₂CO₂H-p as test precursor were similar to the controls. (e) Attempts were made to isolate the penicillin. With N-allyl- β -chloropropionamide as precursor the active material was recovered as the Na salt, 900 units/mg., distribution coefficient 0.64, but Cl in the product was below theory. β , β -Diphenylpropionic acid led to a penicillin, 1700 units/mg., coefficient 0.84, containing no diphenylpropionic group, but probably an aliphatic acyl group (UV absorption). Tryparsamide led to no As in the recovered penicillin; similarly, 2-thiophenecarboxylic acid and some derivs. were not utilized. Data obtained by these methods are presented for many compds. including aryl carboxylic acids, α -substituted phenylacetic acids, aliphatic acids, aryl aliphatic (other than acetic) acids, a miscellaneous unclassified group of acids, and derivs. of these acids. Preparation and some properties of new compds. in the above series are presented. Methods of preparation were: (A) The Schotten-Baumann method was applied to the acid chloride and the amino compound, allylamine, HOCH₂CH₂NH₂, or DL-valine. (B) The Et or Me ester was heated with the amine. (C) EtSH (40 g.) was allowed to react with CH₂:CHCO₂Me (43 g.) in the presence of Triton B (2 drops) to form EtSCH₂CH₂CO₂Me (61 g.), b₅₅ 109-13°. (D) CH₂:CHCH₂SCH₂CONHCH₂CH₂OH (Soper, et al. J. Am. Chemical Society 70, 2849-55(1948)) (53.0 g.) in 100 mL. Me₂CO was treated with 33.0

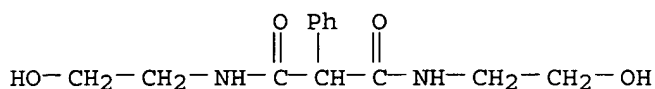
mL. 30% H₂O₂ for 1 wk. N-2-hydroxyethyl- α -(allylsulfinyl)acetamide (II) was recrystd. from EtOAc or EtOAc-MeOH. (E) CH₂:CHCH₂SCH₂CONHCH₂CH₂OH (44.5 g.) in 1 l. Me₂CO with 75 mL. 30% H₂O₂ was allowed to stand 10 days yielding 47.4 g. of the sulfonyl compound (III), an orange oil. (F) Addition of CH₂:CHCOOMe (100 g.) to 200 mL. CH₂:CHCH₂OH, in which was dissolved 5.3 g. Na, produced a gelatinous precipitate. The mixture was heated 1 h., poured into water, and extracted with ether. The ether solution was dried and distilled, b₆₅ 116-32°, n_{20.5D} 1.4312, yield 50.3 g., mainly Me β -(allyloxy)propionate. The 2nd fraction b₆₅ 120-30°, n_{20.5D} 1.4394, yield 23.5 g., was chiefly the allyl ester. (G) DL-Alanyl-DL-valine (Fischer and Scheibler, C.A. 3, 315) was treated with p-ClC₆H₄COCl and NaOH to give about 90% N-[N-(p-chlorobenzoyl)-DL-alanyl]-DL-valine (IV), m. 204-6° (from dilute EtOH). p-ClC₆H₄CO₂H contaminant was removed by washing with ether. (H) CH.tplbond.CCMe₂OH (Hurd and McPhee, C.A. 41, 4095g) (130 g.), CuO (10 g.), NH₄Cl (5 g.) and concentrated HCl (225 mL.) were shaken together 0.5 h. below 40°, and the non-aqueous layer washed with HCl, dried, and fractionated to yield 34% CH.tplbond.CCMe₂Cl, b. 77-9° (Favorskii and Favorskaya, C.A. 39, 3651.4). This compound (194 g.) was treated with malonic ester (330 g.) in 1 l. absolute alc. in which had been dissolved 46 g. Na, the mixture filtered, the alc. evaporated under vacuum, the residual sirup treated with dilute cold HCl, extracted with ether, the ether solution washed and dried, the ether evaporated, and the remaining liquid fractionated in vacuo through a Vigreux column to give 192 g. (45%) CH.tplbond.CCMe₂CH(CO₂Et)₂, b₃ 102-4°; from this was derived 148 g. (98%) of the crystalline acid, m. 105-6°. The acid was decarboxylated by heating at 180-200° 1-2 h. to 85% CH.tplbond.CCMe₂CH₂CO₂H (IVa), b₂ 75-7° (bath temperature 130°); Me ester b. 150-3°, 65% yield. (I) Chloroacetylvaline (9.4 g.) was added to 10 g. PhAsCl₂ in 30 mL. 10 N NaOH (Quick and Adams, C.A. 16, 1560). After dilution, filtering, and acidification, an oil precipitated which on recrystn. from water gave 8.5 g. CHMe₂CH(COOH)NHC(=O)CH₂.As(O₂H)Ph (V), m. 188° (decomposition). (J) To the Grignard reagent from m-(CF₃)C₆H₄Br, Mg, and dry ether 0.15 g. powdered Se was added (Morgan and Porritt, C.A. 19, 3260) and the mixture hydrolyzed. After the ether layer was separated, washed, and extracted with 3 N NaOH, the resulting aqueous extract was added to 0.15 mol ClCH₂CO₂Na in 100 mL. water. In a few min. the mixture was acidified. Alternate extns. with ether and alkaline solution and acidification gave m-(CF₃)C₆H₄SeCH₂CO₂H (Va) b₇ 140-2°, m. 58.5-9.5°. (K) Cl(CH₂)₃CN (52 g.), PhSH (56 g.), and NaOMe (28 g.) in 300 mL. absolute alc. was refluxed with stirring overnight. After the solvent was evaporated, the organic layer was washed and distilled in vacuo to give 72 g. impure PhS(CH₂)₃CN b_{0.1} 135-7°; the acid obtained on hydrolysis m. 58-60°. (L) Br(CH₂)₄CO₂Et, PhSH, and NaOEt in absolute alc. produced PhS(CH₂)₄CO₂Et, b_{0.2} 121-4°. (M) HO₂C(CH₂)₄CO₂Et (87 g.) with SOCl₂ formed the chloride, which with PhCl, AlCl₃, and CS₂ gave 66.4 g. p-ClC₆H₄CO(CH₂)₄CO₂Et, m. 59-60°; saponification with KOH gave the acid, m. 134-6°. Reduction with Zn and HCl in toluene-water, followed by treatment with MeOH resulted in p-ClC₆H₄(CH₂)₅CO₂Me, b_{0.4} 122-5°. (N) (p-ClC₆H₄)₂CO was converted by the Reformatskii reaction to 90% (p-ClC₆H₄)₂C(OH)CH₂CO₂Et, m. 96-7°, dehydrated by P₂O₅ in C₆H₆ and saponified to (p-ClC₆H₄)₂C:CHCO₂H, m. 173-4°. The acid was allowed to take up 0.10 mol H at 4 atmospheric over 5% Pd on C to yield 71% (p-ClC₆H₄)₂CHCH₂CO₂H (VI), m. 182-3°. (O) Desoxyanisoin and BrCH₂CO₂Et in dry C₆H₆ was treated with Zn dust, the reaction mixture shaken

with dilute H₂SO₄, the C₆H₆ layer separated and dried, and, after removal of the

C₆H₆, the product distilled in vacuo with dehydration to 90% Et
 β,γ -bis(p-methoxyphenyl)butenoate, b₂ 221°;
 hydrogenation and saponification gave 90% β,γ -bis(p-methoxyphenyl)butyric acid (VII), m. 167-8°. Data on precursors are given in the order: acid, N-substituted amide, method of preparation (or taken from the literature or purchased com.), m.p. or b.p. of amide, stimulation (see Test a) of the amide (if no amide is given, value is for the acid): NCCH₂CO₂H, HOCH₂CH₂, B, oil, 0.9; ClCH₂CH₂CO₂H, allyl, A, 39-40°, 1.0; HOCH₂CH₂CO₂H, HOCH₂CH₂, B, 73.5-75, 1.0; γ,γ,γ -trichlorobutyric, DL-valine, A, 197, 1.0; CF₃CH(OH)CH₂CO₂H, HOCH₂CH₂, B, 59-61, 1.1; CH₂:CHCH₂CO₂H, HOCH₂CH₂, A, b₁ 138-42, 1.4; (ethylmercurimercapto)acetic, -, -, -, toxic; β -hydroxybutyric, HOCH₂CH₂, B, 68-71, 1.0; MeOCH₂CH₂CO₂H, HOCH₂CH₂, B, b₁ 142-5, 1.0; 2-thiophenecarboxylic (VIII), HOCH₂CH₂, B, 90-1, 1.0; VIII, allyl, A, 65, 1.0; VIII, DL-valine, A, 123-4, 1.0; allylsulfinylacetic, II, D, 81.5-82, 1.2; allylsulfonylacetic, III, E, oil, 0.9; EtSCH₂CH₂CO₂H (C), HOCH₂CH₂, B, b₀.45 173-5, 1.0; sorbic, HOCH₂CH₂, B, b₁ 158-60, 1.1; β -allyloxypropionic (F), HOCH₂CH₂, B, b₀.3 142-4, 0.8; tert-butylacetic, DL-valine, A, 147-8, 0.8; isocaproic, DL-valine, A, 100-1, 1.0; γ -ethoxybutyric, HOCH₂CH₂, B, b₁ 138-40, 1.0; p-ClC₆H₄CO₂H (IX), HOCH₂CH₂, A, 113-14, 1.0 (acid alone, 1.0); IX, allyl, A, 73, 1.0; IX, DL-valine, A, 178-9, 1.0; IX, DL-alanyl-DL-valine, G, 204-6, 1.0; BzOH (X), allyl, -, -, 0.9; X, 2-benzamido-1,3-propanediol, B, 67-9, 1.0; p-O:AsC₆H₄CH₂CO₂H, -, -, -, 1.0; PhCH₂SO₂H, DL-valine, A, 120-3, 1.0; IVa, (H), HOCH₂CH₂, B, b₀.5 150-5, 0.8; cyclopentylacetic, HOCH₂CH₂, B, 57-8, 1.6; hexahydrobenzoic, DL-valine, A, 195-7, 1.0; BzCO₂H, -, -, -, 1.0; mandelic, HOCH₂CH₂, B, 61-4, 1.0; PhSeCH₂CO₂H, HOCH₂CH₂, A, 56-8, 1.2 (acid alone, 1.8); PhSO₂CH₂CO₂H, HOCH₂CH₂, B, 93-4, 1.1 (acid alone, 1.0); Ph(HO₂)AsCH₂CO₂H, DL-valine, I, 188 (dec.), 1.0 (acid alone, toxic); C₆H₁₁CH₂CO₂H (XI), HOCH₂CH₂, B, 66-8, 1.0; XI, DL-valine, A, 178-9, 1.1; δ -carbethoxyvaleric, HOCH₂CH₂, A, oil, 1.0; PhC.tplbond.CCO₂H, -, -, -, 0.9; NCCHPhCO₂H, HOCH₂CH₂, B, 105-7, 0.8; Va, -, J, 58.5-9.5, 1.0; cinnamic (XII), HOCH₂CH₂, B, 101, 1.0; XII, DL-valine, A, 183-4, 1.0; XII, allyl, A, 90-2, 0.9; (2,4-dichlorobenzylsulfonyl)acetic, -, -, -, 0.9; PhCH(CO₂H)₂, bis(2-hydroxyethyl), B, oil, 1.2; (p-chlorobenzylsulfonyl)acetic, -, -, -, 0.9; hydrocinnamic, DL-valine, A, 141-3, 1.0; MeCH(SPh)CO₂H, -, -, -, 1.3; PhSCH₂CH₂CO₂H, DL-valine, A, 93-4, 1.1; MeOCHPhCO₂H, HOCH₂CH₂, B, 84-7, 1.0; tropic, HOCH₂CH₂, B, oil, 1.2; PhCH₂SO₂CO₂H, -, -, -, 1.0; N-phenylsarcosine, HOCH₂CH₂, B, 56-7, 1.0; (p-chlorocarbobenzoxy)glycine, -, -, 108-9.5, 1.0; γ -(2,4-dichlorophenoxy)butyric, -, -, -, toxic; styrylacetic, allyl, A, 61-3, 1.4; β -(p-bromophenyl)butyric, DL-valine, A, 134-5, 2.5; carbobenzoxyglycine, -, -, -, 1.2; γ -(p-nitrophenyl)butyric, DL-valine, A, 138-43, 1.5; EtCHPhCO₂H, DL-valine, A, oil, 1.0; Me₂CPhCO₂H, DL-valine, A, oil, 1.1; β -phenylbutyric, HOCH₂CH₂, B, oil, 0.9; γ -phenylmercaptobutyric, -, K, 58-60, 2.0; γ -phenoxybutyric, HOCH₂CH₂, B, 70-2, 1.0; γ -(p-aminophenyl)butyric, DL-valine, obtained by catalytic hydrogenation of the nitro compound, 175-9, 0.8; fencholic, -, -, -, toxic; γ -cyclohexylbutyric, HOCH₂CH₂, B, 45-8, 1.1; capric, HOCH₂CH₂, -, 75, 1.0; 3-indolepropionic, -, -, -, 0.9; γ -benzoylbutyric, -, -, -, 1.0; benzylsuccinic, -, -, -, 1.0; γ -(p-bromophenyl)isovaleric, DL-valine, A, 109-10, 0.8; β -(p-chlorophenyl)isovaleric, -, -, -, 0.5; β -(p-fluorophenyl)isovaleric, -, -, -, 0.9; β -(p-iodophenyl)isovaleric, -, -, -, toxic; β -(p-nitrophenyl)isovaleric, DL-valine, A, 110-15, 1.3; δ -phenylvaleric, DL-valine, A, 98-100, 0.8; δ -phenylmercaptovaleric (L), HOCH₂CH₂, B, 91-2, 1.0; β -(p-

hydroxyphenyl)isovaleric, -, -, -, 1.0; β -(p-aminophenyl)isovaleric, -, -, -, 1.0; p-Me₃SiC₆H₄SeCH₂CO₂H, -, -, b4 170-3, toxic; cyclohexylvaleric, -, -, -, toxic; 10-hendecenoic, HOCH₂CH₂, B, 66-7, 1.0; 3-indolebutyric, HOCH₂CH₂, B, oil, 1.0; ϵ -(p-chlorophenyl)caproic (M), HOCH₂CH₂, B, oil, 1.4; lauric, HOCH₂CH₂, B, 86-7, 0.9; 1-naphthalenepropionic, HOCH₂CH₂, B, 60-1, 1.0; 6-benzoyl-3-ketocaproic, -, -, -, 1.0; γ -mesitylbutyric, -, -, 82-4, toxic (acid); Ph₂CHCO₂H, HOCH₂CH₂, B, 118-19, 1.0; myristic, HOCH₂CH₂, B, 94-5, 1.0; VI (N), DL-valine, A, 155-6, 0.9 (acid alone 0.4); Ph₂CHCH₂CO₂H, HOCH₂CH₂, B, 94, 0.9; 4-methoxy-1-naphthalenebutyric, HOCH₂CH₂, B, oil, 0.6; (PhCH₂)₂CHCO₂H, HOCH₂CH₂, B, 83-4, 0.9; palmitic, HOCH₂CH₂, B, 97.5, 1.0; β , β -di-p-tolylpropionic, HOCH₂CH₂, B, 85-6, 0.9; 9-(p-iodophenyl)hendecanoic, HOCH₂CH₂, B, oil, 1.0; 3-phenylhendecanoic, HOCH₂CH₂, B, oil, 1.0; linoleic, HOCH₂CH₂, B, b1 215-20, 0.9; VII (O), DL-valine, A, 147-8, 1.0; ricinoleic, HOCH₂CH₂, B, 54-5, 1.0; 9,10-dihydroxystearic, HOCH₂CH₂, B, 150, 1.4; β -1-pyrenoylpropionic (C₂₀H₁₄O₃), -, -, -, toxic.

IT 860374-08-9, Malonamide, N,N'-bis(2-hydroxyethyl)-2-phenyl-
(in penicillin production)
RN 860374-08-9 HCAPLUS
CN Malonamide, N,N'-bis(2-hydroxyethyl)-2-phenyl- (5CI) (CA INDEX NAME)



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FILE CONTENT:1840 - 4 Dec 2005 VOL 143 ISS 23

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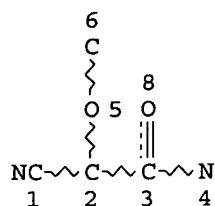
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L1 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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STEREO ATTRIBUTES: NONE
 L36 2 SEA FILE=CASREACT SSS FUL L1 (35 REACTIONS)

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L36 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 142:23494 CASREACT
 TITLE: Three-Component Condensation Leading to β -Amino
 Acid Diamides: Convergent Assembly of β -Peptide
 Analogues
 AUTHOR(S): Oaksmith, Jennifer M.; Peters, Ulf; Ganem, Bruce
 CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Baker
 Laboratory, Cornell University, Ithaca, NY,
 14853-1301, USA
 SOURCE: Journal of the American Chemical Society (2004),
 126(42), 13606-13607
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A Passerini condensation of acyl cyanides, carboxylic acids, and
 isonitriles has been developed that affords efficient access to
 functionalized diamides as well as β -peptides of α -hydroxy-
 β -amino acids. Such compds. are protease-resistant and form stable
 helical and sheet structures when incorporated into larger peptides (no
 data given). N-Protected α -amino acids and isocyanoesters derived
 from α -amino acids participate in the condensation, leading to
 α/β peptides embodying the heterogeneous $\alpha/\beta/\alpha$
 backbone motif.

RX(1) OF 45 A + B + C ==> D...

RX(1) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO D 799778-66-8
NTE no solvent, Passerini condensation

RX(2) OF 45 E + B + C ==> F...

RX(2) RCT E 58040-74-7, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO F 799778-69-1
NTE no solvent, Passerini condensation

RX(3) OF 45 G + B + C ==> H

RX(3) RCT G 68077-52-1, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO H 799778-72-6
NTE no solvent, Passerini condensation

RX(4) OF 45 I + B + C ==> J

RX(4) RCT I 42867-40-3, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO J 799778-75-9

NTE no solvent, Passerini condensation

RX(5) OF 45 K + B + C ==> L

RX(5) RCT K 799779-56-9, B 64-19-7

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)

RCT C 931-53-3

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO L 799778-78-2

NTE no solvent, Passerini condensation

RX(6) OF 45 A + M + C ==> N

RX(6) RCT A 631-57-2, M 124-07-2

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)

RCT C 931-53-3

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO N 799778-83-9

NTE no solvent, Passerini condensation

RX(7) OF 45 E + M + C ==> O...

RX(7) RCT E 58040-74-7, M 124-07-2

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)

RCT C 931-53-3

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO O 799778-85-1

NTE no solvent, Passerini condensation

RX(8) OF 45 A + B + P ==> Q...

RX(8) RCT A 631-57-2, B 64-19-7

STAGE(1)

Sackey 10_673988

CON 10 minutes, 0 deg C

STAGE(2)

RCT P 7188-38-7

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO Q 799778-93-1

NTE no solvent, Passerini condensation

RX(9) OF 45 E + B + P ==> R

RX(9) RCT E 58040-74-7, B 64-19-7

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)

RCT P 7188-38-7

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO R 799778-98-6

NTE no solvent, Passerini condensation

RX(10) OF 45 A + B + S ==> T

RX(10) RCT A 631-57-2, B 64-19-7

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)

RCT S 2769-64-4

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO T 799779-07-0

NTE no solvent, Passerini condensation

RX(11) OF 45 A + B + U ==> V

RX(11) RCT A 631-57-2, B 64-19-7

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)

RCT U 2999-46-4

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

PRO V 799779-11-6

NTE no solvent, Passerini condensation

RX(12) OF 45 A + B + W ==> X...

RX(12) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT W 43219-50-7
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO X 799779-16-1
NTE no solvent, Passerini condensation

RX(13) OF 45 I + M + W ==> Y

RX(13) RCT I 42867-40-3, M 124-07-2

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT W 43219-50-7
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO Y 799779-19-4
NTE no solvent, Passerini condensation

RX(14) OF 45 A + B + Z ==> AA...

RX(14) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT Z 799779-64-9
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO AA 799779-25-2
NTE no solvent, Passerini condensation

RX(15) OF 45 A + B + AB ==> AC

RX(15) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)

RCT AB 799779-66-1
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO AC 799779-28-5
NTE no solvent, Passerini condensation

RX(16) OF 45 A + AD + C ==> AE

RX(16) RCT A 631-57-2, AD 140-10-3, C 931-53-3
PRO AE 799778-81-7
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(17) OF 45 G + AG + C ==> AH

RX(17) RCT G 68077-52-1, AG 501-52-0, C 931-53-3
PRO AH 799778-88-4
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(18) OF 45 E + AI + C ==> AJ

RX(18) RCT E 58040-74-7, AI 65-85-0, C 931-53-3
PRO AJ 799778-90-8
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(19) OF 45 A + AK + P ==> AL

RX(19) RCT A 631-57-2, AK 1161-13-3, P 7188-38-7
PRO AL 799779-01-4
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(20) OF 45 A + AM + P ==> AN...

RX(20) RCT A 631-57-2, AM 13734-34-4, P 7188-38-7
 PRO AN 799779-04-7
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 12 hours, room temperature
 NTE Passerini condensation

RX(21) OF 45 K + AI + S ==> AO...

RX(21) RCT K 799779-56-9, AI 65-85-0, S 2769-64-4
 PRO AO 799779-09-2
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 12 hours, room temperature
 NTE Passerini condensation

RX(22) OF 45 K + AG + U ==> AP...

RX(22) RCT K 799779-56-9, AG 501-52-0, U 2999-46-4
 PRO AP 799779-13-8
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 12 hours, room temperature
 NTE Passerini condensation

RX(23) OF 45 A + AK + Z ==> AQ

RX(23) RCT A 631-57-2, AK 1161-13-3, Z 799779-64-9
 PRO AQ 799779-22-9
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 12 hours, room temperature
 NTE Passerini condensation

RX(24) OF 45 A + AM + Z ==> AR...

RX(24) RCT A 631-57-2, AM 13734-34-4, Z 799779-64-9
 PRO AR 799779-30-9
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 12 hours, room temperature
 NTE Passerini condensation

RX(25) OF 45 ...D ==> AS

RX(25) RCT D 799778-66-8

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 22 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO AS 799779-32-1
NTE stage 1 chemoselective

RX(26) OF 45 ...2 F + AX ==> AY + AZ

RX(26) RCT F 799778-69-1, AX 67-56-1

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 46 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO AY 799779-35-4, AZ 851165-95-2
NTE stage 1 chemoselective

RX(27) OF 45 ...0 ==> BA

RX(27) RCT O 799778-85-1

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 46 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BA 799779-37-6
NTE stage 1 chemoselective

RX(28) OF 45 ...Q ==> BB

RX(28) RCT Q 799778-93-1

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 23 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BB 799779-39-8
NTE stage 1 chemoselective, alternate one-pot two-step synthesis shown

RX(29) OF 45 ...AO ==> BC

RX(29) RCT AO 799779-09-2

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 46 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BC 799779-43-4
NTE stage 1 chemoselective

RX(30) OF 45 ...2 AP + 2 AX ==> BD + BE

RX(30) RCT AP 799779-13-8, AX 67-56-1

• STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 22 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BD 799779-45-6, BE 851166-00-2
NTE stage 1 chemoselective

RX(31) OF 45 ...X ==> BF

RX(31) RCT X 799779-16-1

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 23 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BF 799779-47-8
NTE stage 1 chemoselective

RX(32) OF 45 ...AA ==> BG

RX(32) RCT AA 799779-25-2

STAGE(1)

RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 16 hours, room temperature

STAGE(2)

RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)

RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BG 799779-49-0
NTE stage 1 chemoselective

RX(33) OF 45 ...AN ==> BH

RX(33) RCT AN 799779-04-7
RGT AU 1333-74-0 H2
PRO BH 799779-41-2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 16 hours, room temperature
NTE chemoselective, product depends on solvent

RX(34) OF 45 ...AR ==> BJ

RX(34) RCT AR 799779-30-9
RGT AU 1333-74-0 H2
PRO BJ 799779-50-3
CAT 7440-05-3 Pd, 7440-02-0 Ni
SOL 109-99-9 THF
CON 25 hours, room temperature
NTE chemoselective, product depends on solvent, Raney nickel used
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 135:152562 CASREACT
TITLE: Dehydration method for producing 2-
(alkoxy)malonodinitriles from 2-alkoxymalondiamides
INVENTOR(S): Bartek, Johannes; Fuchs, Rudolf; Hildbrand, Stefan
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 13 pp.

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058857	A1	20010816	WO 2001-EP1505	20010209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US, US, US RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001033759	A5	20010820	AU 2001-33759	20010209
EP 1254105	A1	20021106	EP 2001-905765	20010209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003522753	T2	20030729	JP 2001-558409	20010209
US 2003144538	A1	20030731	US 2002-182716	20021011
US 6673957	B2	20040106		
US 2004063987	A1	20040401	US 2003-673988	20030930
PRIORITY APPLN. INFO.:			EP 2000-102758	20000210
			EP 2000-109505	20000504
			US 2001-267087P	20010207
			WO 2001-EP1505	20010209
			US 2002-182716	20021011

OTHER SOURCE(S): MARPAT 135:152562

AB 2-(Alkoxy)malonodinitriles (NC)2CHOR (R = C1-6 alkyl, halogen-substituted C1-6 alkyl) (e.g., 2-methoxymalonodinitrile) or 2-(alkoxy)-2-cyanoacetamides are prepared by the dehydration of the corresponding 2-alkoxymalondiamides (H2NCO)2CHOR in the presence of a dehydrating agent (e.g., POCl3).

RX(2) OF 2 A ==> F

RX(2) RCT A 5018-31-5
 RGT C 10025-87-3 POCl3
 PRO F 353291-71-1
 CAT 7446-70-0 AlCl3
 SOL 75-05-8 MeCN

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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